

Introduction to MHD Simulation

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Goal

- To understand basic ideas of MHD simulation
- Introductory course
- Many simple/sample/example codes.
- I'll make the source codes available for you.
 - Check my lab's website:
URL: <http://www.research.kobe-u.ac.jp/csi-viz/>
 - The lecture note (this pdf file) will be available, too
at the above URL and this school's web page.

Outline

- Speed of computers
- How can we make use of computer's speed?
- Numerical methods
- Sample 1-D simulations

TOP500 List

TOP500 List - November 2010 (1-100)

R_{max} and R_{peak} values are in TFlops. For more details about other fields, check the [TOP500 description](#).

Power data in KW for entire system

URL: <http://www.top500.org/list/2010/11/100>

Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	National Supercomputing Center in Tianjin China	Tianhe-1A - NUDT TH MPP, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C / 2010 NUDT	186368	2566.00	4701.00	4040.00
2	DOE/SC/Oak Ridge National Laboratory United States	Jaguar - Cray XT5-HE Opteron 6-core 2.6 GHz / 2009 Cray Inc.	224162	1759.00	2331.00	6950.60
3	National Supercomputing Centre in Shenzhen (NSCS) China	Nebulae - Dawning TC3600 Blade, Intel X5650, Nvidia Tesla C2050 GPU / 2010 Dawning	120640	1271.00	2984.30	2580.00
4	GSIC Center, Tokyo Institute of Technology Japan	TSUBAME 2.0 - HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows / 2010 NEC/HP	73278	1192.00	2287.63	1398.61
5	DOE/SC/LBNL/NERSC United States	Hopper - Cray XE6 12-core 2.1 GHz / 2010 Cray Inc.	153408	1054.00	1288.63	2910.00
6	Commissariat a l'Energie Atomique (CEA) France	Tera-100 - Bull bullex super-node S6010/S6030 / 2010 Bull SA	138368	1050.00	1254.55	4590.00
7	DOE/NNSA/LANL United States	Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband / 2009 IBM	122400	1042.00	1375.78	2345.50
8	National Institute for Computational Sciences/University of Tennessee United States	Kraken XT5 - Cray XT5-HE Opteron 6-core 2.6 GHz / 2009 Cray Inc.	98928	831.70	1028.85	3090.00
9	Forschungszentrum Juelich (FZJ) Germany	JUGENE - Blue Gene/P Solution / 2009 IBM	294912	825.50	1002.70	2268.00
10	DOE/NNSA/LANL/SNL United States	Cielo - Cray XE6 8-core 2.4 GHz / 2010 Cray Inc.	107152	816.60	1028.66	2950.00

FLOPS

- FLOPS
 - = Floating Point number Operations Per Second
- 4700 TFLOPS
- = 4.7 PFLOPS
- = 4.7×10^{15} FLOPS

What is floating point number

- Double precision (64 bit)
 - 1 bit for sign.
 - 11 bits for exponent.
 - 52 bits for mantissa.

$$2^{52} \sim 10^{15.6}$$

- π in double precision floating point

$$\pi = 3.14159265358979$$

What is “operation” in FLOPS?

- Addition (subtraction) and multiplication (division)
- An example of floating point operation:
 - To calculate the floating point number of π^2

$$\begin{aligned}\pi^2 &= 3.14159265358979 \times 3.14159265358979 \\ &= ?\end{aligned}$$

What is Your FLOPS value?

- Using only a pen, paper and your brain...

$$\pi^2 = 3.14159265358979$$

$$\times 3.14159265358979$$

$$?.????????????????$$

- How many seconds do you need?

Top 003 Brain FLOPS

---An International Contest---

#	Name	Country	FLOPS
1			
2			
3			

What is Your FLOPS value?

- How many seconds did you need?
- (For example) 1000 seconds?
-then, you are a **0.001 FLOPS** computer.
- 1 mFLOPS (...not Mega FLOPS)

Human brain as a computer

If a person

- has 0.001 FLOPS speed,
- lives for 100 years,
- devotes the entire life (without sleep) to the floating point number operations (multiplication/addition),

then how many operations could be done in the life work?

Human brain as a computer

If a person

- has 0.001 FLOPS speed,
- lives for 100 years,
- devotes the entire life (without sleep) to the floating point number operations (multiplication/addition),

then how many operations could be done in the life work?

$$\left[100 \text{ years} = 3 \times 10^9 \text{ seconds} \right] \times 0.001$$

Only 3 million operations.

How about the speed of PCs?

- Example: Leibniz formula for pi.

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} = \frac{1}{1} - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \dots = \frac{\pi}{4}$$

leibniz.f90

```
program leibniz
    implicit none
    integer, parameter :: SP = kind(1.0)
    integer, parameter :: DP = selected_real_kind(2*precision(1.0_SP))
    real(DP) :: sign = -1.0_DP
    real(DP) :: sum = 0.0_DP
    integer :: odd_int

    do odd_int = 2*(10**6)+1 , 1 , -2
        sign = sign * (-1.0_DP)
        sum = sum + sign/odd_int
    end do

    print *, ' 4*sum = ', 4*sum
end program leibniz
```

Code:

- src/CountFlops/

leibniz.f90

```
program leibniz
    implicit none
    integer, parameter :: SP = kind(1.0)
    integer, parameter :: DP = selected_real_kind(2*precision(1.0_SP))
    real(DP) :: sign = -1.0_DP
    real(DP) :: sum = 0.0_DP
    integer :: i
    do i= 2*(10**6)+1 , 1 , -2
        sign = sign*(-1.0_DP)
        sum = sum + sign/i
    end do
    print *, ' 4*sum = ', 4*sum
end program leibniz
```

Repeat for one million times

Odd integers.

multiplication (once)

division (once)

addition (once)

3M Floating Point Operations

- 3 million floating point operations experiment
 - one million time steps.
 - 3 floating point number operations per each step.
- A human brain takes 100 years.
- Let's try.

Result

- 3 million floating point operations experiment
 - one million steps.
 - 3 floating point number operations per each step.
- A human brain takes 100 years.
- ... 0.009 second by this PC.
- $3 \times 10^6 / 9 \times 10^{-3}$ FLOPS
- = 0.3 GFLOPS

Speed contrast

- Our brain = mFLOPS (10^{-3} FLOPS)
- PC = GFLOPS (10^9 FLOPS)
- Supercomputer = 10^{15} FLOPS

Concorde is only 400-500 times faster than our walk speed.



Speed Contrast

- Speed contrast: Supercomputer / PC = 10^6
- Speed contrast: Supercomputer / brain = 10^{18}
 - Human walk = 1-2 m/s
 - Speed of light = 3×10^8 m/s
 - Speed contrast: light / walk = 10^8

The approach of computer simulation

- Your problem (to be solved)
- Convert (or approximate) it into the form with +, -, *, /
- Make computers solve it.

Methods used in MHD simulations

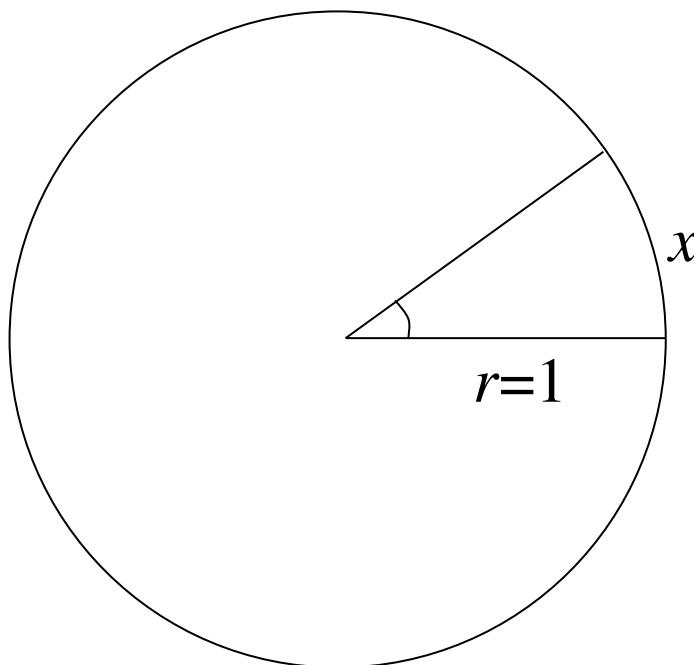
- Spectral methods
- Finite difference method
- Finite volume method
- Finite element method
- . . .

Discretization

- NS eq., MHD equations., etc...
- Continuous x (space) and t (time)
- Differential equations
- Convert the differential Equations
 - ➔ Eqs with +, -, *, /
- “Discretization”

Various numerical method: An explanation through a simple 1-D problem

The diffusion equation on a circle

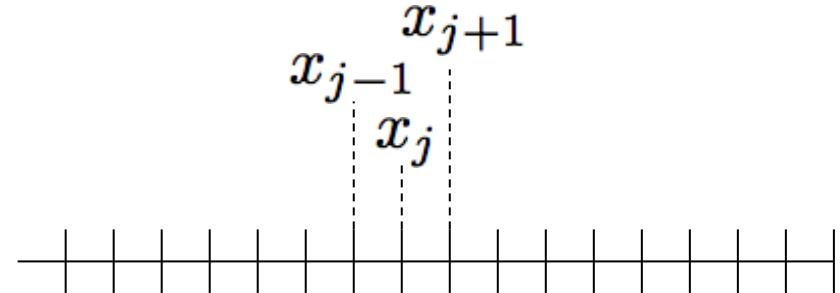


$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

$$0 \leq x < 2\pi$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

(1) FDM: Finite Difference Method



$$\frac{d\psi}{dx} \sim \frac{\psi_{j+1} - \psi_{j-1}}{2\Delta x}$$

$$\frac{d^2\psi}{dx^2} \sim \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta x}$$

$$\frac{d\psi_j}{dt} = \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

(1) FDM: Finite Difference Method

$$\frac{d\psi_j}{dt} = \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}$$

$$\frac{d\psi_j}{dt} = f(\psi_1, \psi_2, \dots, \psi_N)$$

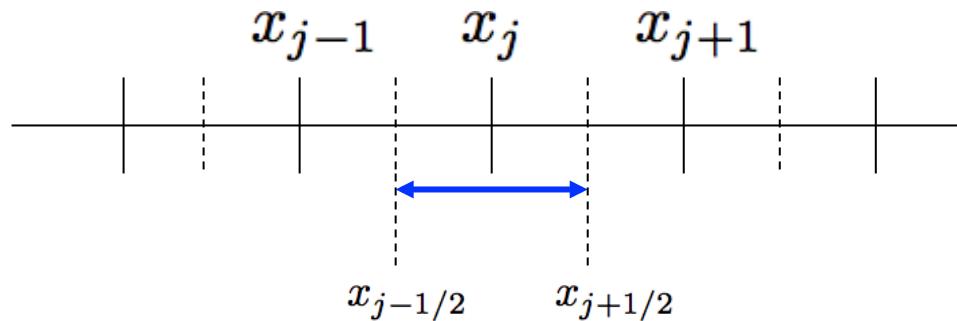
==> Common numerical integrators (e.g., Runge-Kutta).

We will see in practice by this note PC.

$$\boxed{\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}}$$

(2) FVM: Finite Volume Method

$$\rightarrow \quad \frac{\partial \psi}{\partial t} = \frac{\partial F}{\partial x}, \quad F = \frac{\partial \psi}{\partial x}$$



$$\int_{x_{j-1/2}}^{x_{j+1/2}} \frac{\partial \psi}{\partial t} dx = \int_{x_{j-1/2}}^{x_{j+1/2}} \frac{\partial F}{\partial x} dx,$$

cell average $\left(\bar{f} \equiv \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} f dx \right)$

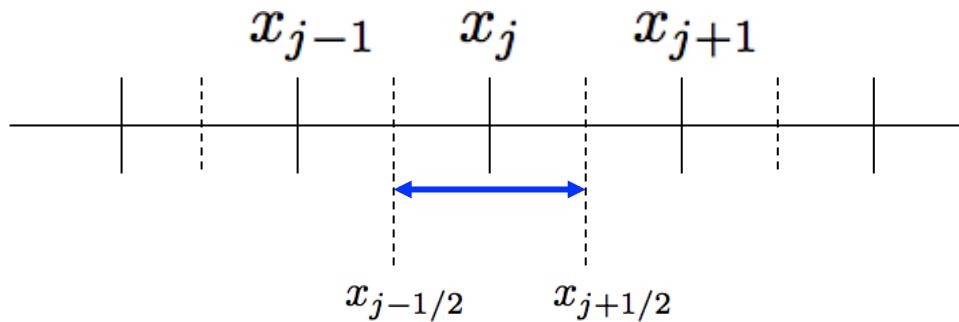
$$\frac{d\bar{\psi}_j}{dt} = [F(x_{j+1/2}) - F(x_{j-1/2})] / \Delta x$$

$$\boxed{\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}}$$

(2) FVM: Finite Volume Method

$$\rightarrow \boxed{\frac{d\bar{\psi}_j}{dt} = [F(x_{j+1/2}) - F(x_{j-1/2})] / \Delta x}$$

$$F = \frac{\partial \psi}{\partial x}$$



$$F(x_{j+1}) = \frac{\bar{\psi}(j+1) - \bar{\psi}(j-1)}{\Delta x}$$



$$\boxed{\frac{d\bar{\psi}_j}{dt} = \frac{\bar{\psi}_{j+1} - 2\bar{\psi}_j + \bar{\psi}_{j-1}}{(\Delta x)^2}}$$

Same as FDM.

$$\boxed{\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}}$$

(3) FEM for 1D diffusion eq.

$\forall a(x)$, (periodic)

$$\int_{-\pi}^{\pi} a(x) \frac{\partial \psi(x)}{\partial x} dx = \int_{-\pi}^{\pi} a(x) \frac{\partial^2 \psi(x)}{\partial x^2} dx$$

$$\boxed{\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}}$$

FEM for 1D diffusion eq.

$\forall a(x)$, (periodic)

$$\begin{aligned} \int_{-\pi}^{\pi} a(x) \frac{\partial \psi(x)}{\partial x} dx &= \int_{-\pi}^{\pi} a(x) \frac{\partial^2 \psi(x)}{\partial x^2} dx \\ &= \left[a \frac{d\psi}{dx} \right]_{-\pi}^{\pi} - \int_{-\pi}^{\pi} \frac{da(x)}{dx} \frac{\partial \psi}{\partial x} dx \end{aligned}$$

$$\boxed{\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}}$$

FEM for 1D diffusion eq.

$\forall a(x)$, (periodic)

$$\int_{-\pi}^{\pi} a(x) \frac{\partial \psi(x)}{\partial x} dx = \int_{-\pi}^{\pi} a(x) \frac{\partial^2 \psi(x)}{\partial x^2} dx$$

$$= \left[a \frac{d\psi}{dx} \right]_{-\pi}^{\pi} - \int_{-\pi}^{\pi} \frac{da(x)}{dx} \frac{\partial \psi}{\partial x} dx$$

$$= - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

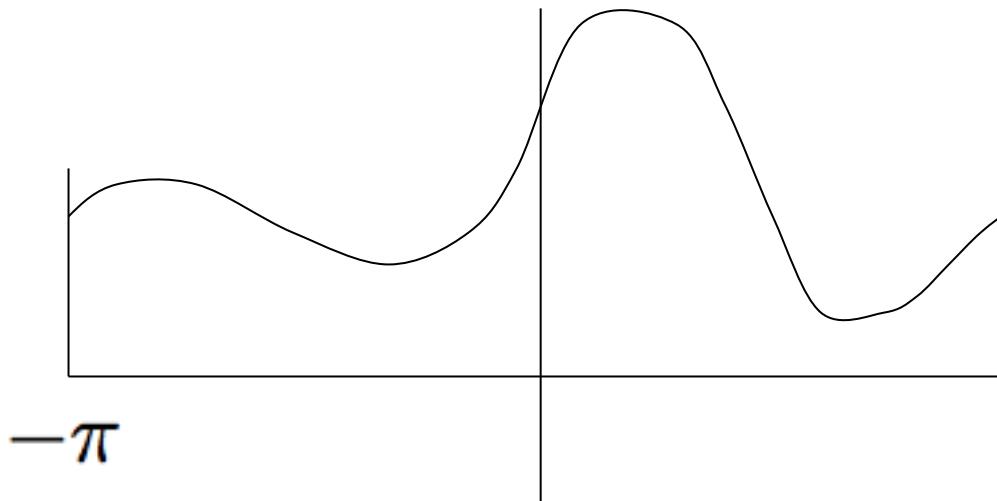
$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

equivalent

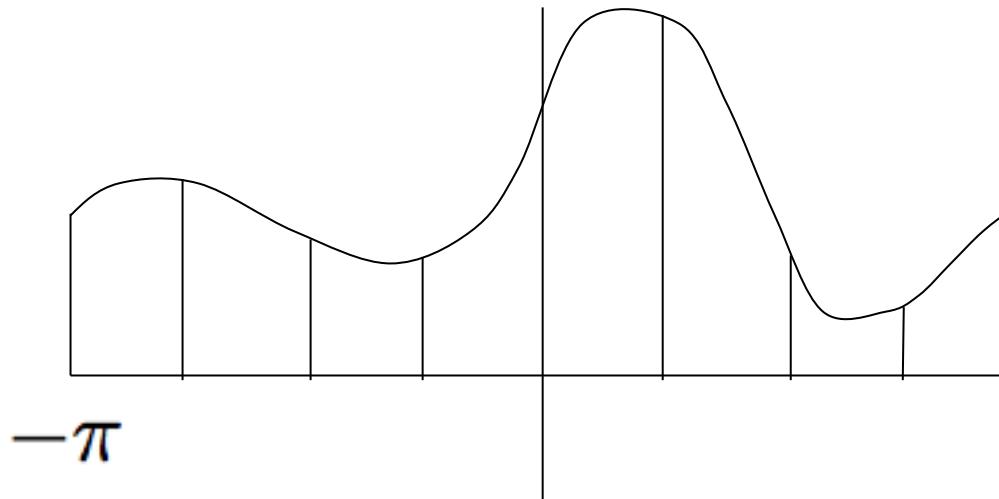
$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$



$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$

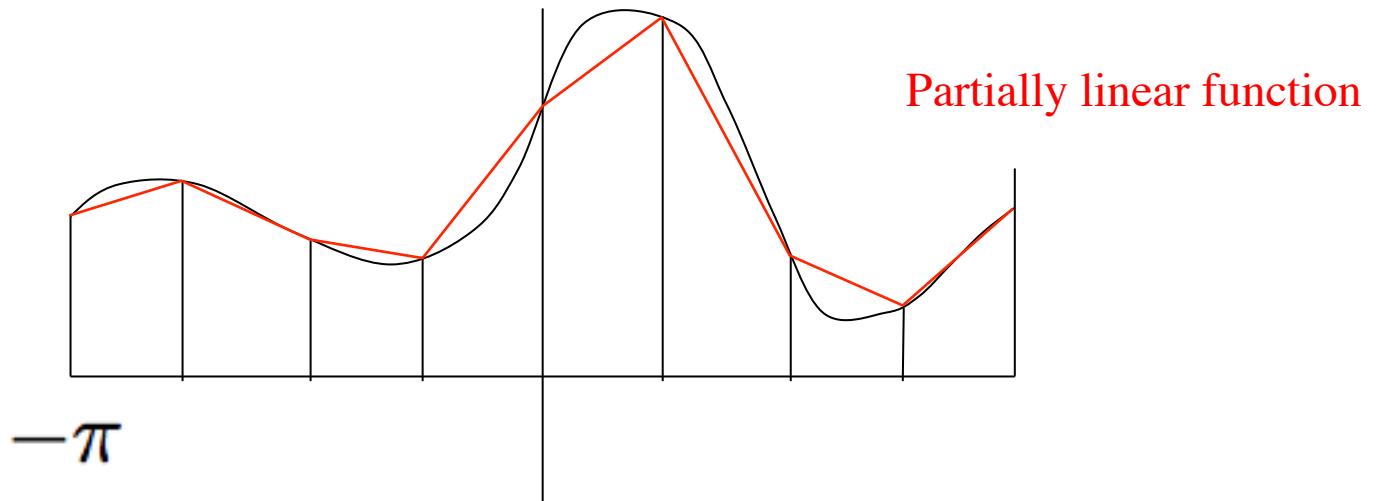


Divide the space x into finite number of sub-spaces (finite element)

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$

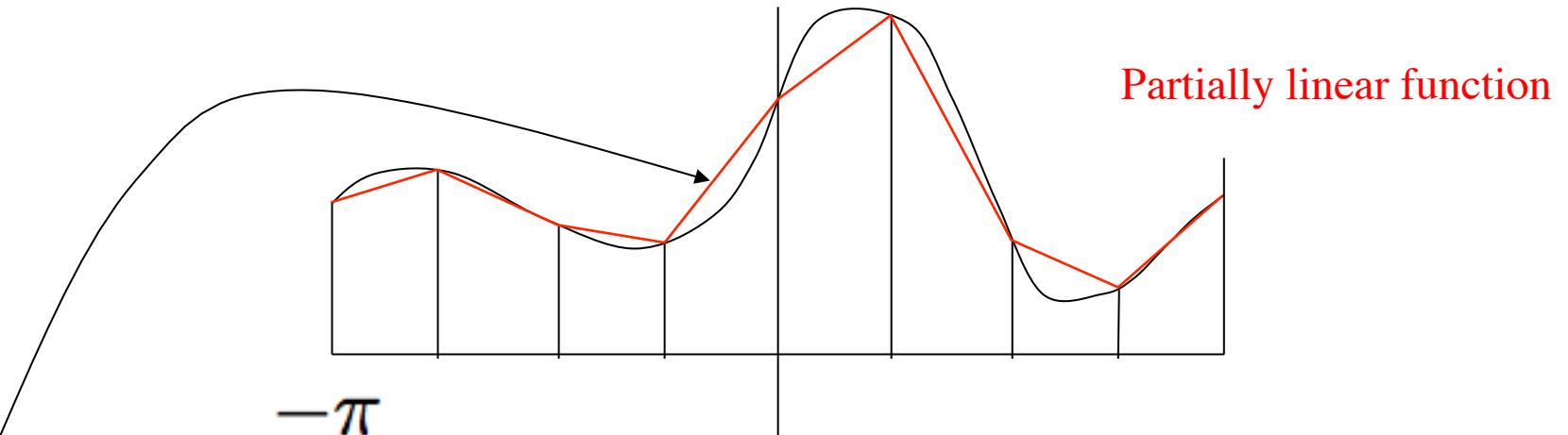


Approximate the function by a partially linear function.

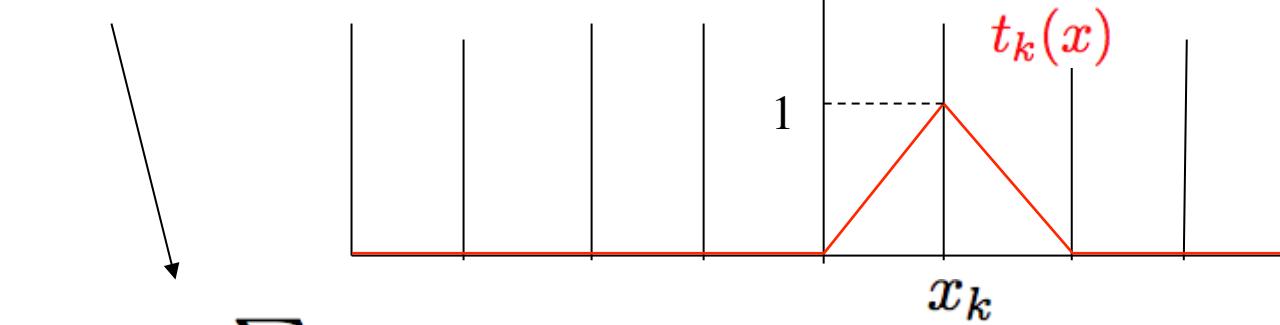
$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$



This profile is expressed by a linear combination of these delta-like (triangle) functions.



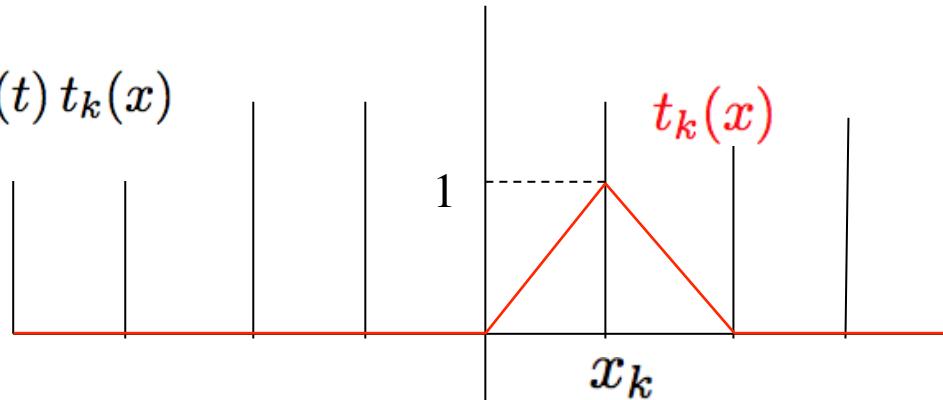
$$\psi(x, t) = \sum_k \psi_k(t) t_k(x)$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

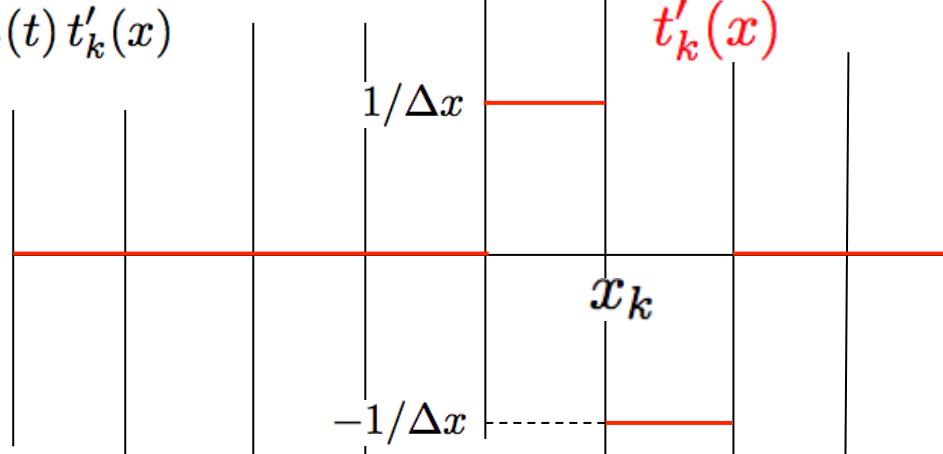
FEM for 1D diffusion eq.

$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$

$$\psi(x, t) = \sum_k \psi_k(t) t_k(x)$$



$$\frac{\partial \psi(x, t)}{\partial x} = \sum_k \psi_k(t) t'_k(x)$$



$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$

Substituting $\psi(x, t) = \sum_k \psi_k(t) t_k(x)$ and $\frac{\partial \psi(x, t)}{\partial x} = \sum_k \psi_k(t) t'_k(x)$

$$\sum_k \frac{d\psi_k(t)}{dt} \int_{-\pi}^{\pi} a(x) t_k(x) dx = - \sum_k \psi_k(t) \int_{-\pi}^{\pi} a'(x) t'_k(x) dx$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

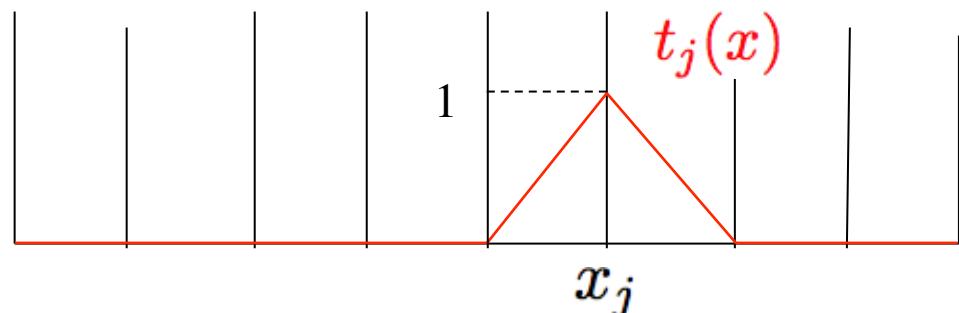
$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$

Substituting $\psi(x, t) = \sum_k \psi_k(t) t_k(x)$ and $\frac{\partial \psi(x, t)}{\partial x} = \sum_k \psi_k(t) t'_k(x)$

$$\sum_k \frac{d\psi_k(t)}{dt} \int_{-\pi}^{\pi} a(x) t_k(x) dx = - \sum_k \psi_k(t) \int_{-\pi}^{\pi} a'(x) t'_k(x) dx$$

Take $a(x) = t_j(x)$, $(j = 1, 2, 3, \dots)$

$a'(x) = t'_j(x)$, $(j = 1, 2, 3, \dots)$



$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\forall a(x), \quad \int_{-\pi}^{\pi} a(x) \frac{\partial \psi}{\partial t} dx = - \int_{-\pi}^{\pi} a'(x) \frac{\partial \psi}{\partial x} dx$$

Substituting $\psi(x, t) = \sum_k \psi_k(t) t_k(x)$ and $\frac{\partial \psi(x, t)}{\partial x} = \sum_k \psi_k(t) t'_k(x)$

$$\sum_k \frac{d\psi_k(t)}{dt} \int_{-\pi}^{\pi} a(x) t_k(x) dx = - \sum_k \psi_k(t) \int_{-\pi}^{\pi} a'(x) t'_k(x) dx$$

Take $a(x) = t_j(x)$, $(j = 1, 2, 3, \dots)$

$a'(x) = t'_j(x)$, $(j = 1, 2, 3, \dots)$

$$\sum_k \frac{d\psi_k(t)}{dt} \underbrace{\int_{-\pi}^{\pi} t_j(x) t_k(x) dx}_{P_{jk}} = - \sum_k \psi_k(t) \underbrace{\int_{-\pi}^{\pi} t'_j(x) t'_k(x) dx}_{Q_{jk}}$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\sum_k P_{jk} \frac{d\psi_k(t)}{dt} = - \sum_k Q_{jk} \psi_k(t)$$

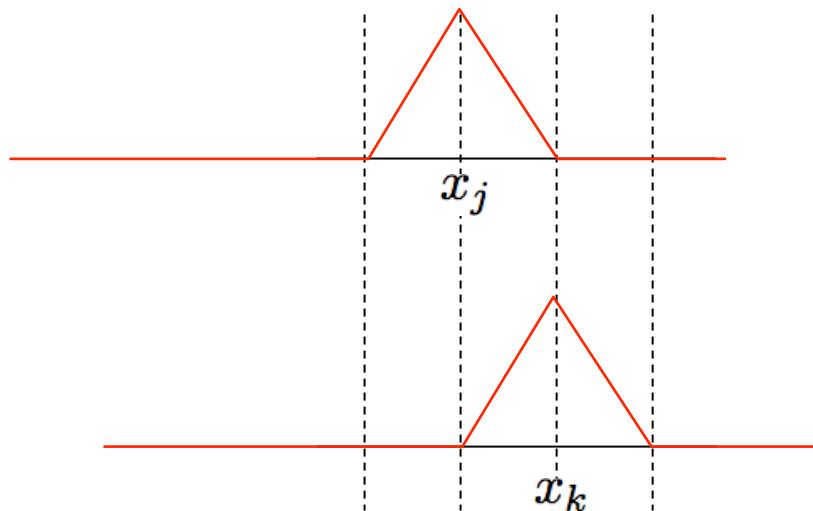
$$P_{jk} = \int_{-\pi}^{\pi} t_j(x) t_k(x) dx \quad Q_{jk} = - \sum_k \psi_k(t) \int_{-\pi}^{\pi} t'_j(x) t'_k(x) dx$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\sum_k P_{jk} \frac{d\psi_k(t)}{dt} = - \sum_k Q_{jk} \psi_k(t)$$

$$P_{jk} = \int_{-\pi}^{\pi} t_j(x) t_k(x) dx = \begin{cases} \frac{2}{3} \Delta x & (j = k) \\ \frac{1}{6} \Delta x & (j = k \pm 1) \\ 0 & (\text{others}) \end{cases}$$

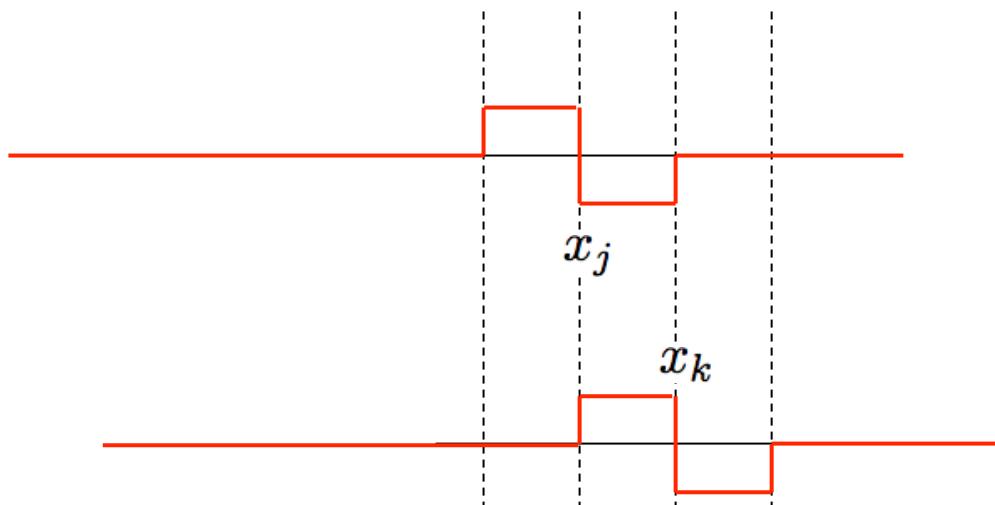


$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\sum_k P_{jk} \frac{d\psi_k(t)}{dt} = - \sum_k Q_{jk} \psi_k(t)$$

$$Q_{jk} = - \sum_k \psi_k(t) \int_{-\pi}^{\pi} t'_j(x) t'_k(x) dx = \begin{cases} \frac{2}{\Delta x} & (j = k) \\ -\frac{1}{\Delta x} & (j = k \pm 1) \\ 0 & (\text{others}) \end{cases}$$



$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$\sum_k P_{jk} \frac{d\psi_k(t)}{dt} = - \sum_k Q_{jk} \psi_k(t)$$

Then this leads to;



$$\frac{1}{6} \left(\frac{d\psi_{j-1}}{dt} + 4 \frac{d\psi_j}{dt} + \frac{d\psi_{j+1}}{dt} \right) = \frac{\psi_{j-1} - 2\psi_j + \psi_{j+1}}{(\Delta x)^2}$$

for $j=2, \dots, N-1$

And with the boundary condition:

$$\frac{d\psi_1}{dt} - \frac{d\psi_{N-1}}{dt} = 0$$

$$\frac{d\psi_N}{dt} - \frac{d\psi_2}{dt} = 0$$

We get a matrix equation as...

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

FEM for 1D diffusion eq.

$$A \mathbf{x} = B \mathbf{y}$$

where (for example, $N=10$ case)

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 1 & 4 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 4 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 4 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 4 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 4 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 4 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad B = \frac{6}{(\Delta x)^2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix}$$

$$\mathbf{x} = \begin{pmatrix} \frac{d\psi_1}{dt} \\ \frac{d\psi_2}{dt} \\ \frac{d\psi_3}{dt} \\ \vdots \\ \frac{d\psi_N}{dt} \end{pmatrix} \quad \mathbf{y} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_N \end{pmatrix}$$

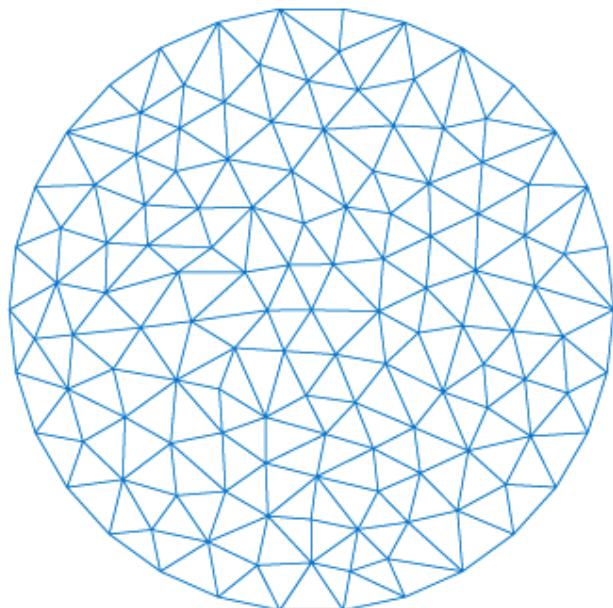
The final step is to solve this matrix eq.

The method depends on how we approximate the time derivative $\frac{d\psi_j}{dt}$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

(3) FEM: Finite Element Method

$$\frac{1}{6} \left(\frac{\psi_{j-1}}{dt} + 4 \frac{d\psi_j}{dt} + \frac{\psi_{j+1}}{dt} \right) = \frac{\psi_{j-1} - 2\psi_j + \psi_{j+1}}{(\Delta x)^2}$$



2D example: Flexible mesh design.

$$\boxed{\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}}$$

(4) Spectral Method

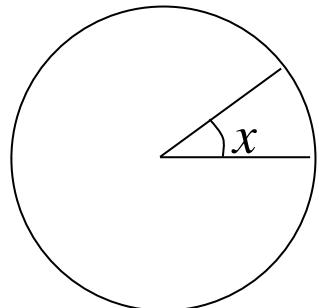
Expansion by a set of orthonormal basis.

$$\psi(x, t) = \sum_k \psi_k(t) a_k(x)$$

$$(a_j, a_k) \equiv \int_{-\pi}^{\pi} a_j^\dagger(x) a_k(x) dx = \delta_{jk}$$

Example: Fourier functions.

$$a_k(x) = \frac{\exp(ikx)}{\sqrt{2\pi}}$$



$$\psi(x, t) = \sum_m \psi_m(t) \frac{\exp(imx)}{\sqrt{2\pi}}$$

$$\rightarrow \frac{\partial^2 \psi(x, t)}{\partial x^2} = - \sum_m m^2 \psi_m(t) \frac{\exp(imx)}{\sqrt{2\pi}}$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

(4) Spectral Method

$$(a_m, \frac{\partial \psi}{\partial t}) = (a_m, \frac{\partial^2 \psi}{\partial x^2})$$

$$\psi(x, t) = \sum_k \psi_k(t) a_k(x)$$

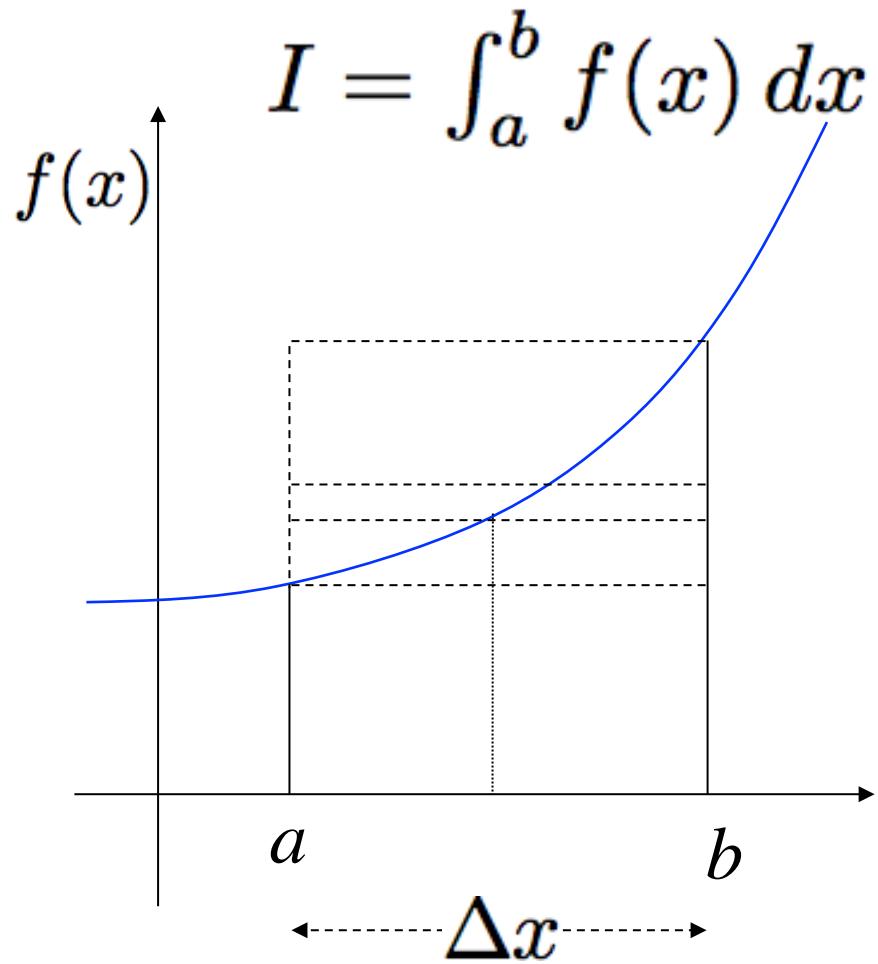
$$\frac{\partial^2 \psi(x, t)}{\partial x^2} = - \sum_k k^2 \psi_k(t) a_k(x)$$

$$(a_j, a_k) = \delta_{jk}$$

$$\frac{d\psi_m(t)}{dt} = -m^2 \psi_m(t)$$

Numerical integration

Numerical integration



1)

$$I = \Delta x f(a)$$

Error $\propto O(\Delta x^2)$

2) Trapezoid rule

$$I = \frac{\Delta x}{2} [f(a) + f(b)]$$

Error $\propto O(\Delta x^3)$

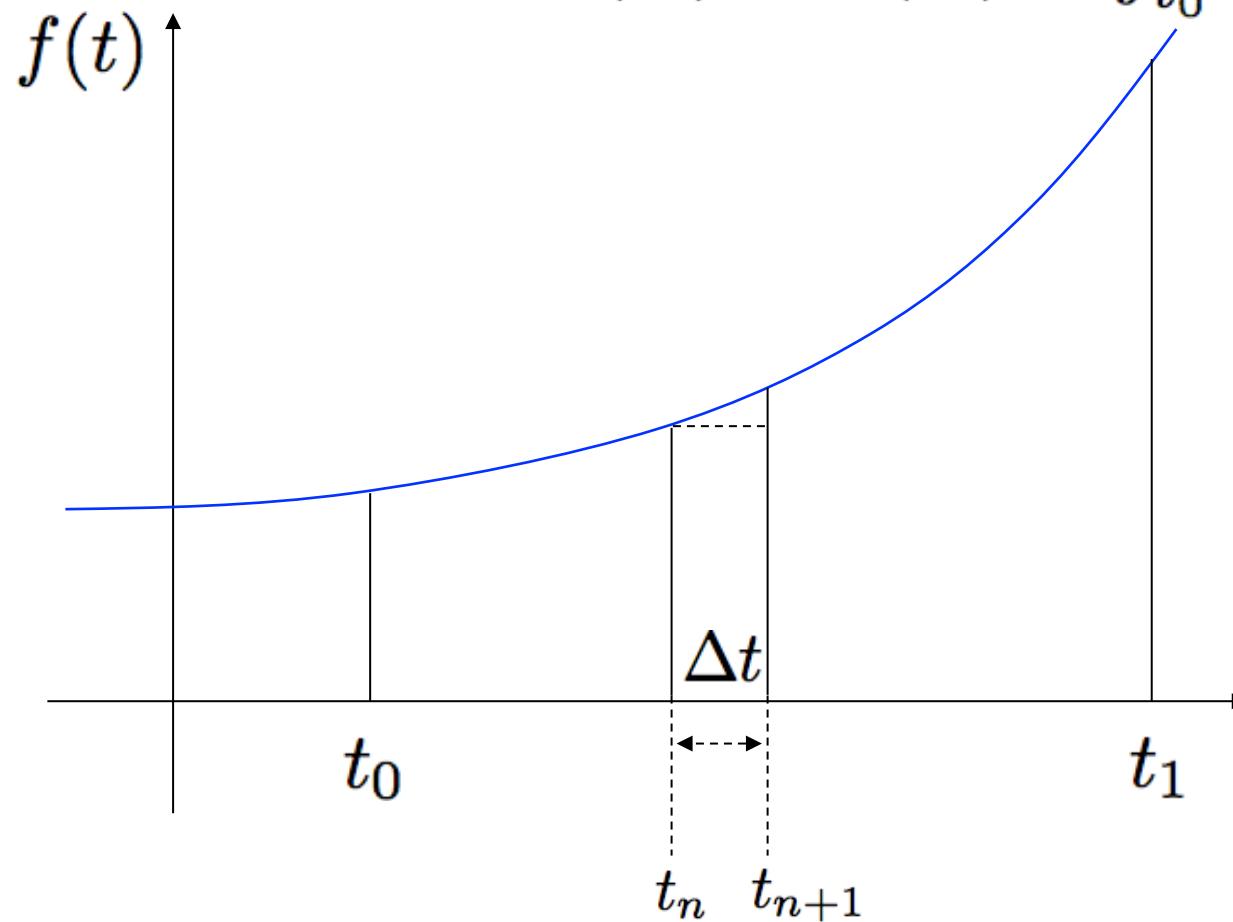
3) Simpson's rule

$$I = \frac{\Delta x}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

Error $\propto O(\Delta x^5)$

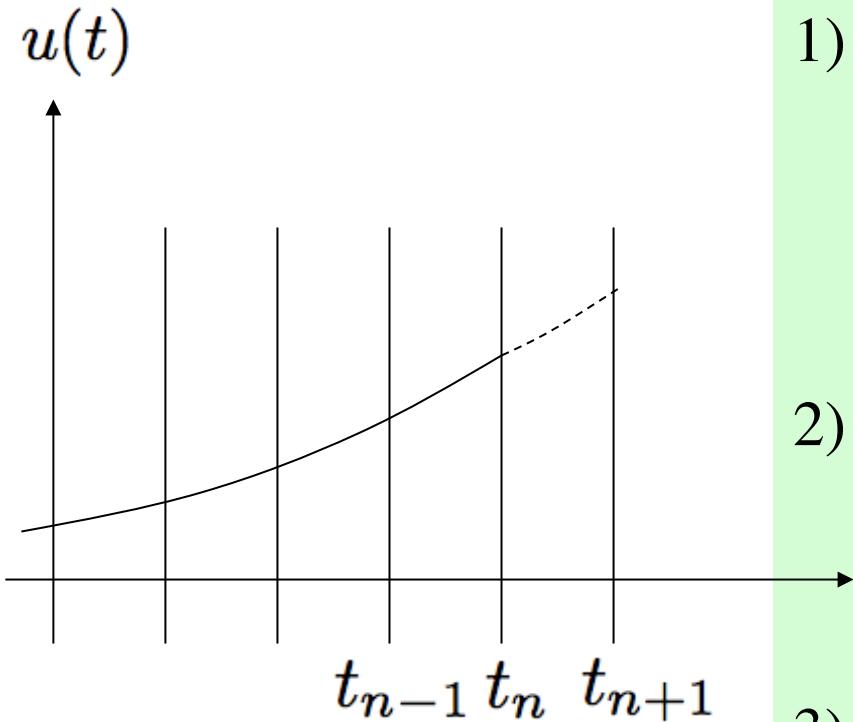
$$\frac{du(t)}{dt} = f(u(t), t)$$

$$u(t_1) = u(t_0) + \int_{t_0}^{t_1} f dt$$



$$\frac{du(t)}{dt} = f(u(t), t)$$

$$u(t_{n+1}) = u(t_n) + \int_{t_n}^{t_{n+1}} f dt$$



1)

$$u(t_{n+1}) = u(t_n) + \Delta t f(t_n)$$

→ 1st order Euler method

2) Trapezoid rule

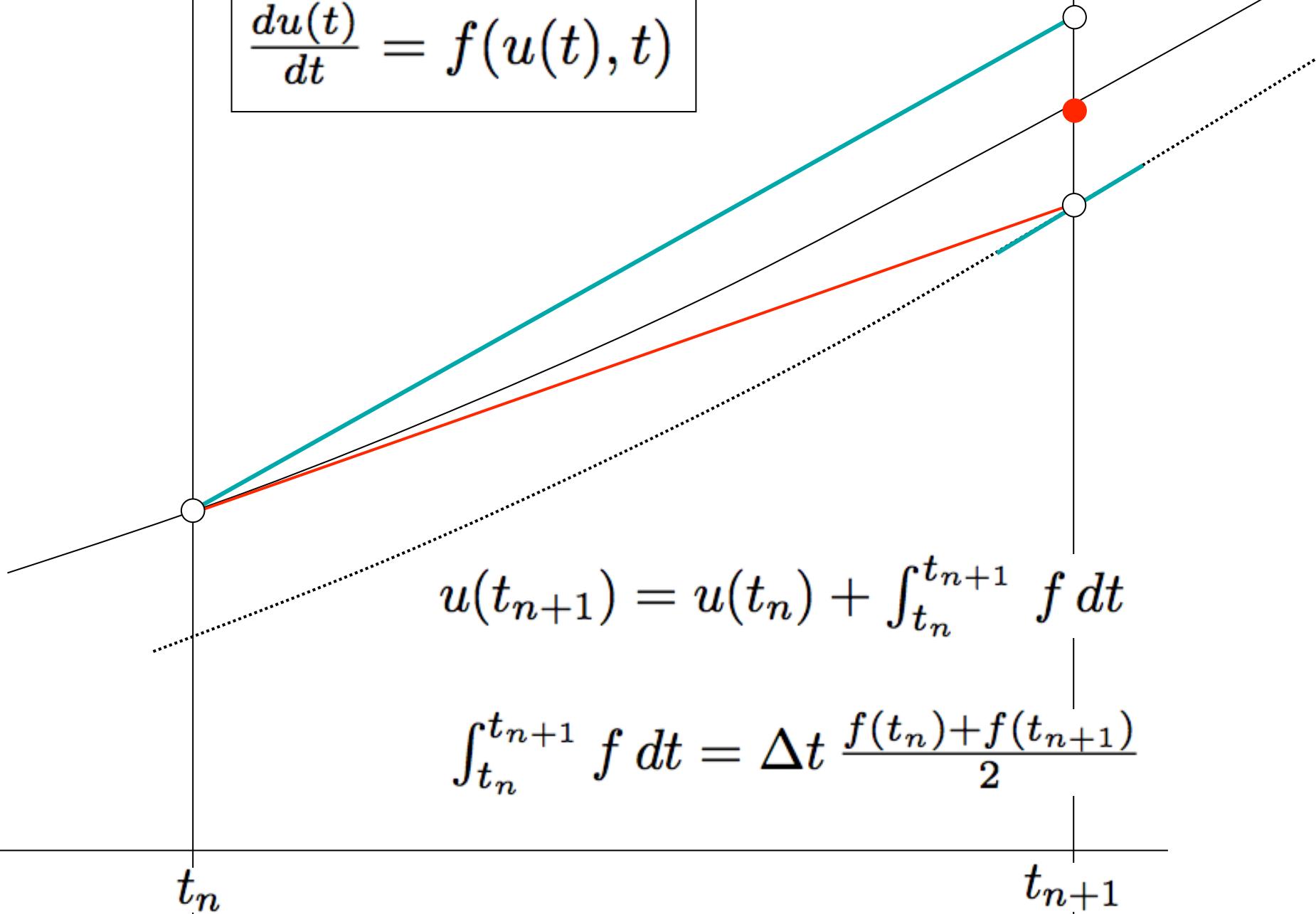
→ 2nd order Runge-Kutta method

3) Simpson's rule

→ 4th order Runge-Kutta method

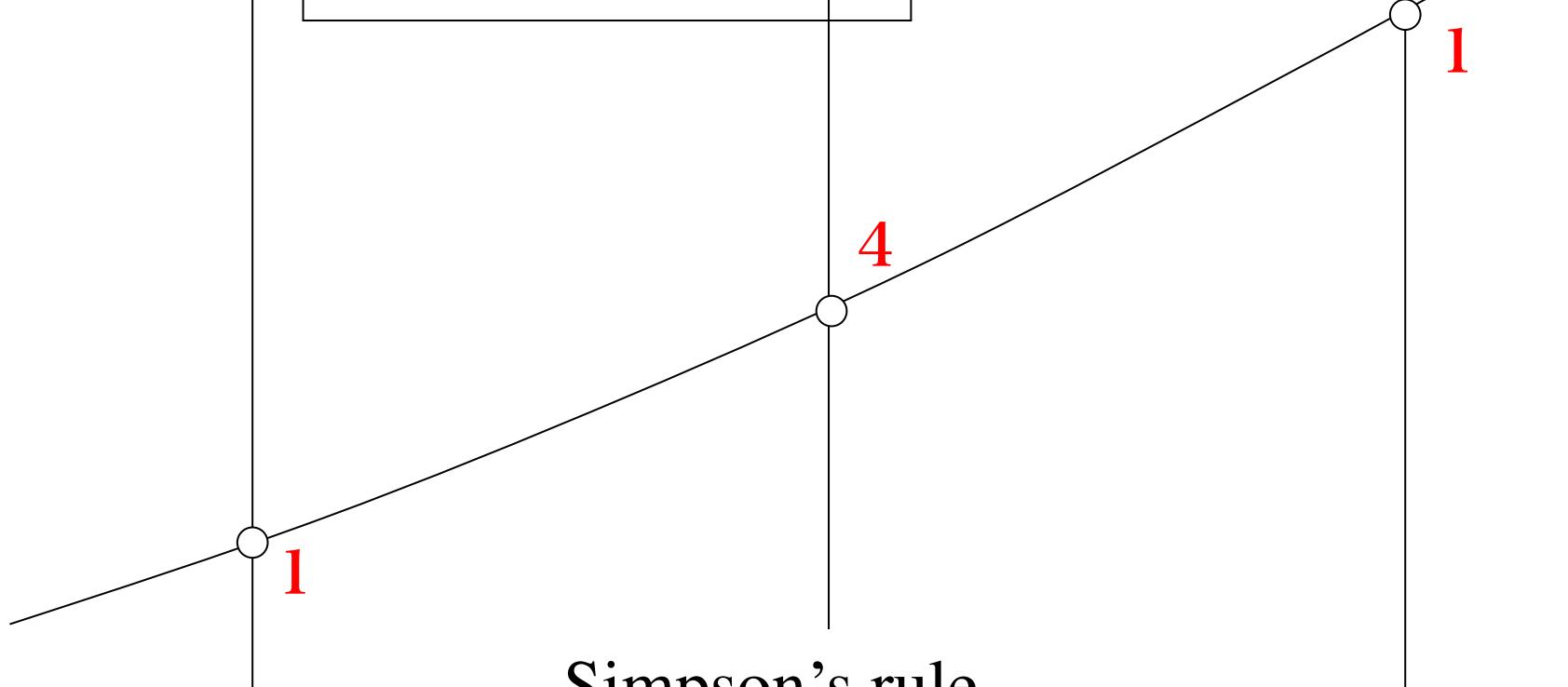
$u(t)$

$$\frac{du(t)}{dt} = f(u(t), t)$$



$u(t)$

$$\frac{du(t)}{dt} = f(u(t), t)$$



Simpson's rule

$$\int_{x_n}^{x_{n+1}} F(x) dx = \frac{(x_{n+1} - x_n)}{6} \left[F(x_n) + 4F\left(\frac{x_n + x_{n+1}}{2}\right) + F(x_{n+1}) \right]$$

$u(t)$

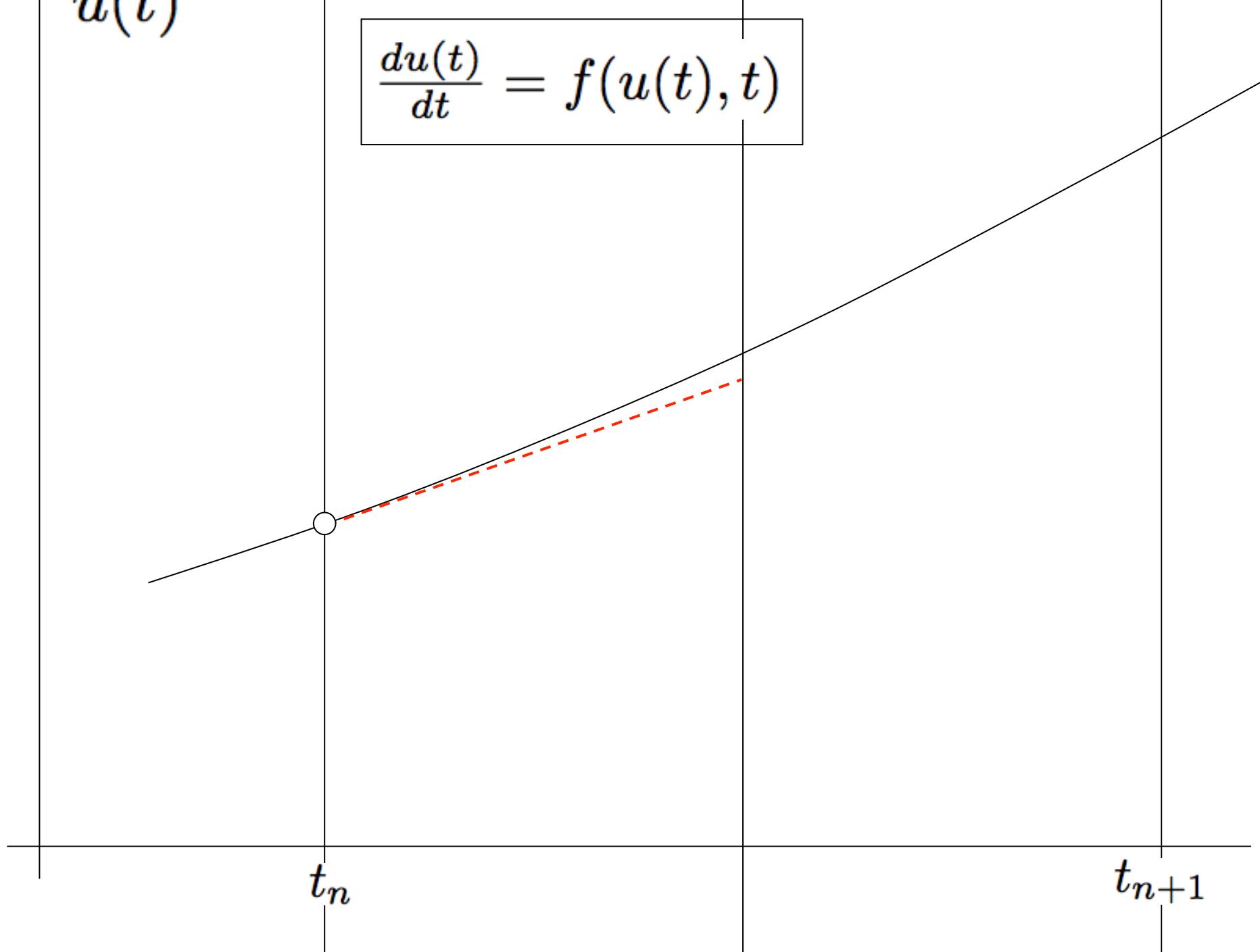
$$\frac{du(t)}{dt} = f(u(t), t)$$

t_n

t_{n+1}

$u(t)$

$$\frac{du(t)}{dt} = f(u(t), t)$$

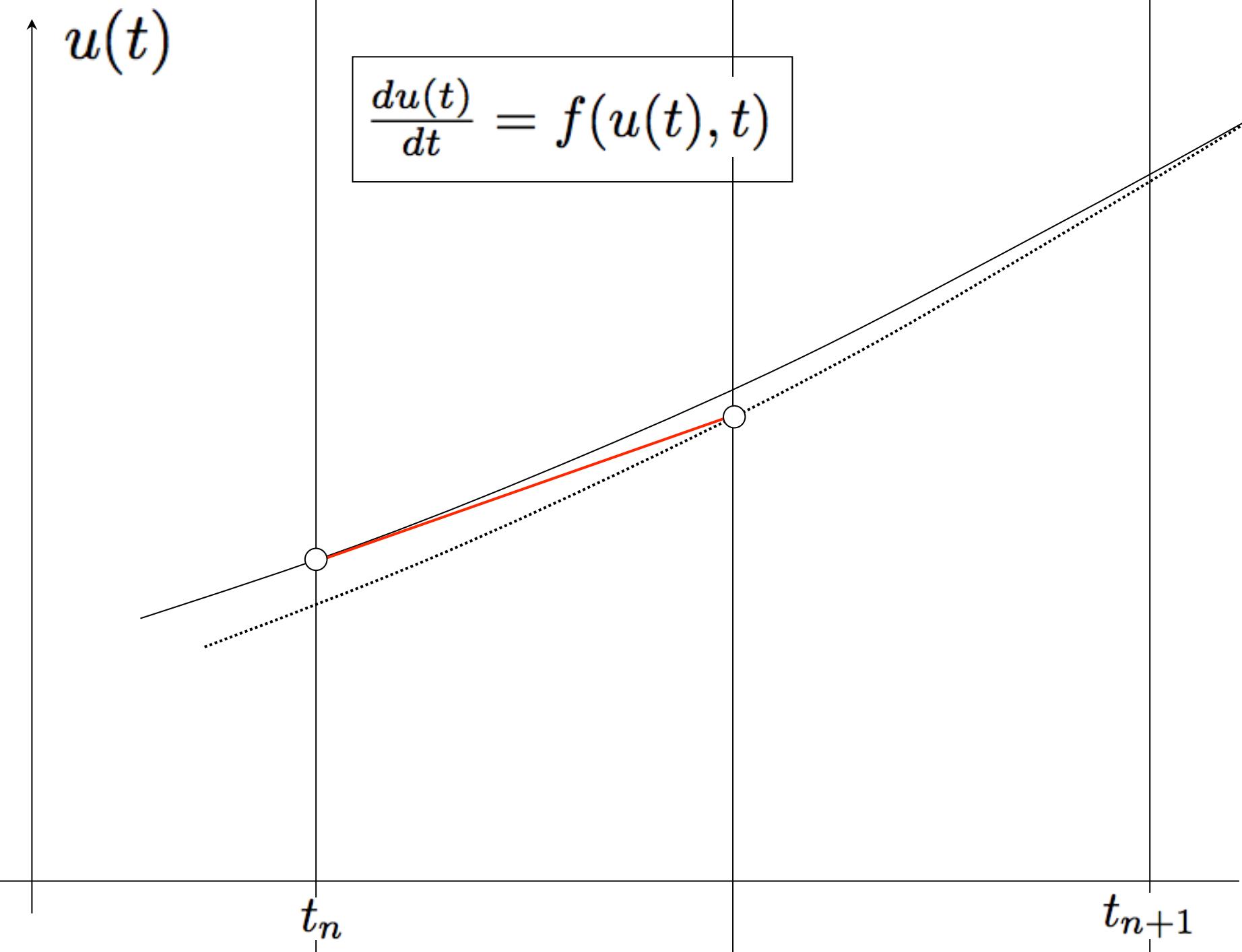


$u(t)$

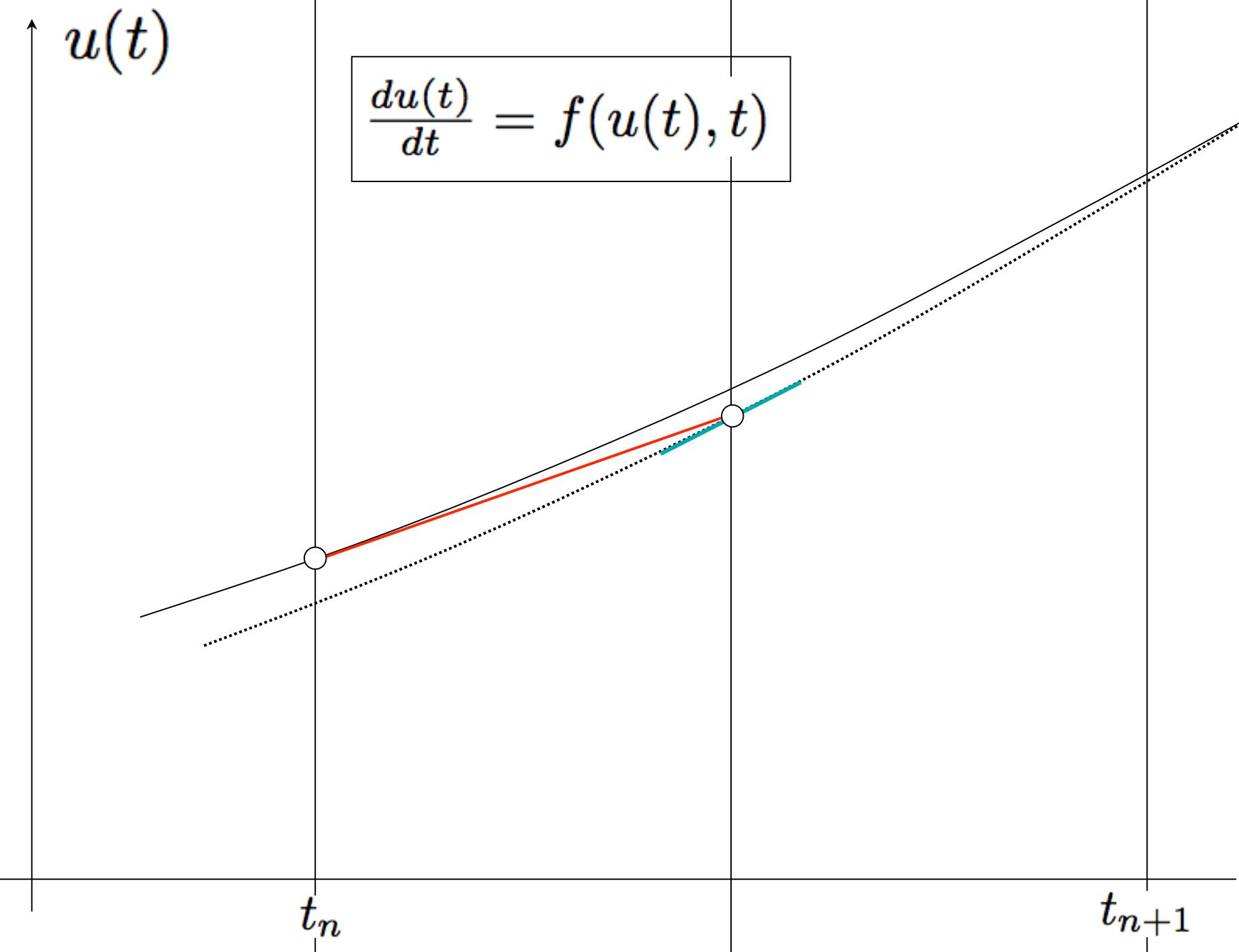
$$\frac{du(t)}{dt} = f(u(t), t)$$

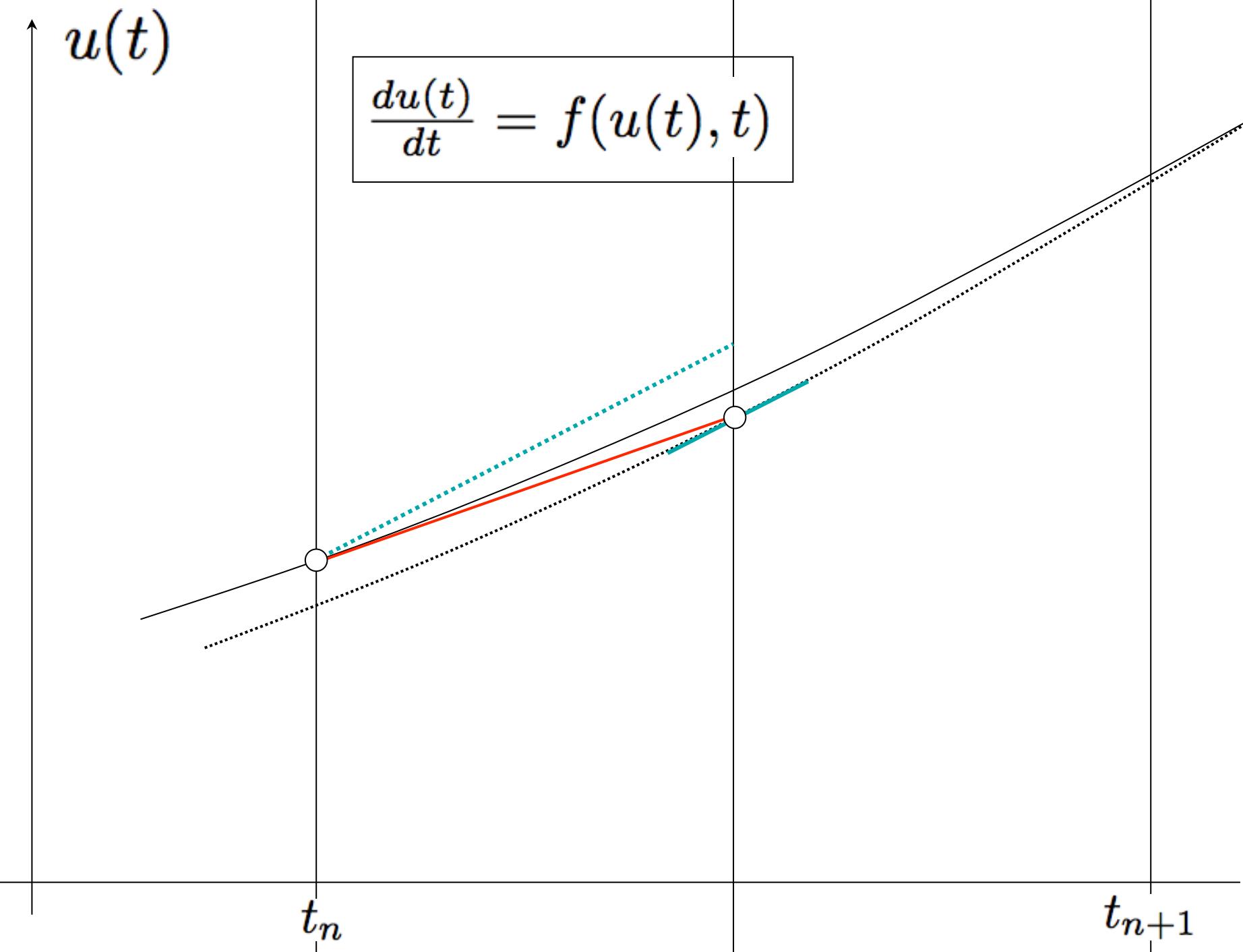
t_n

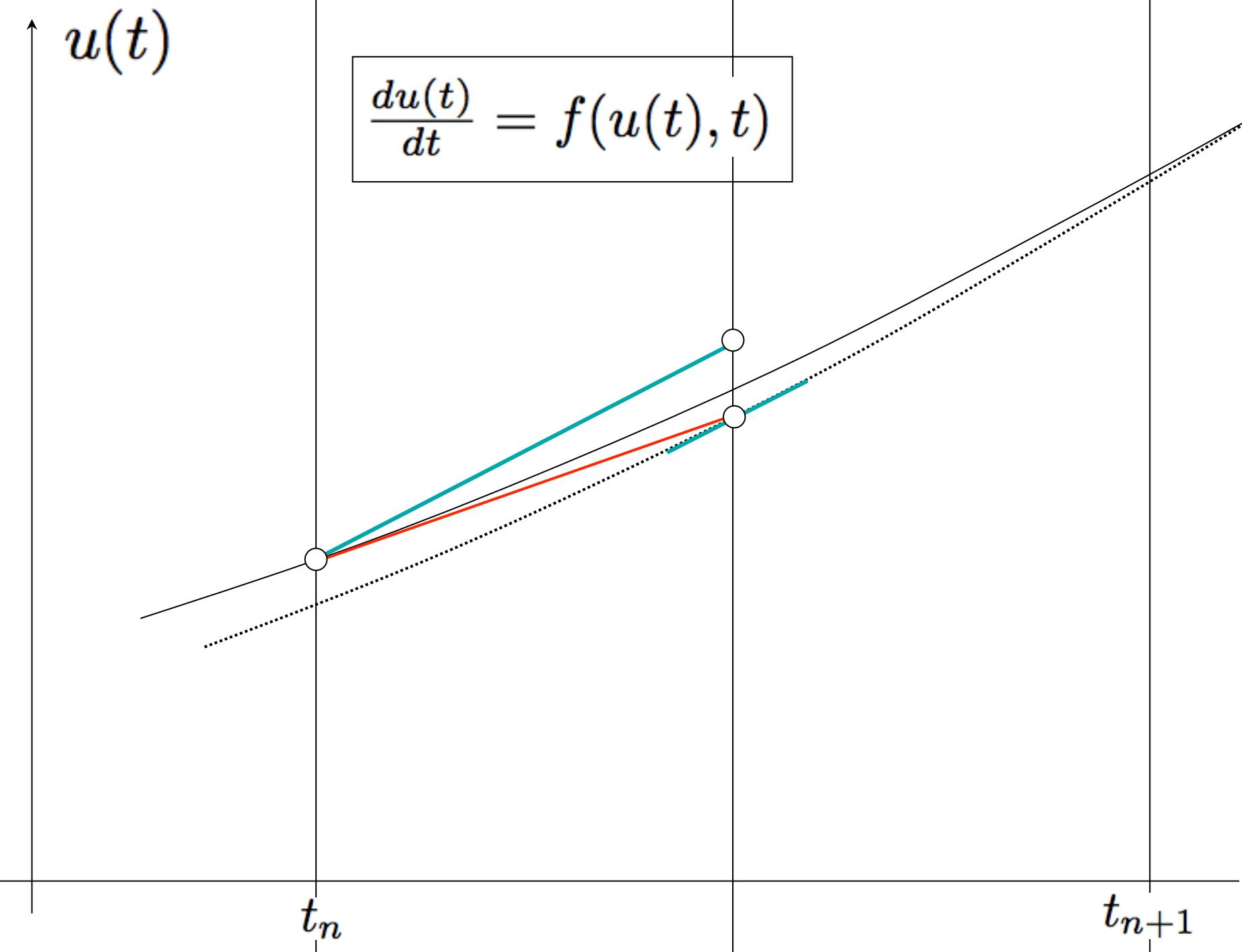
t_{n+1}



$$\frac{du(t)}{dt} = f(u(t), t)$$

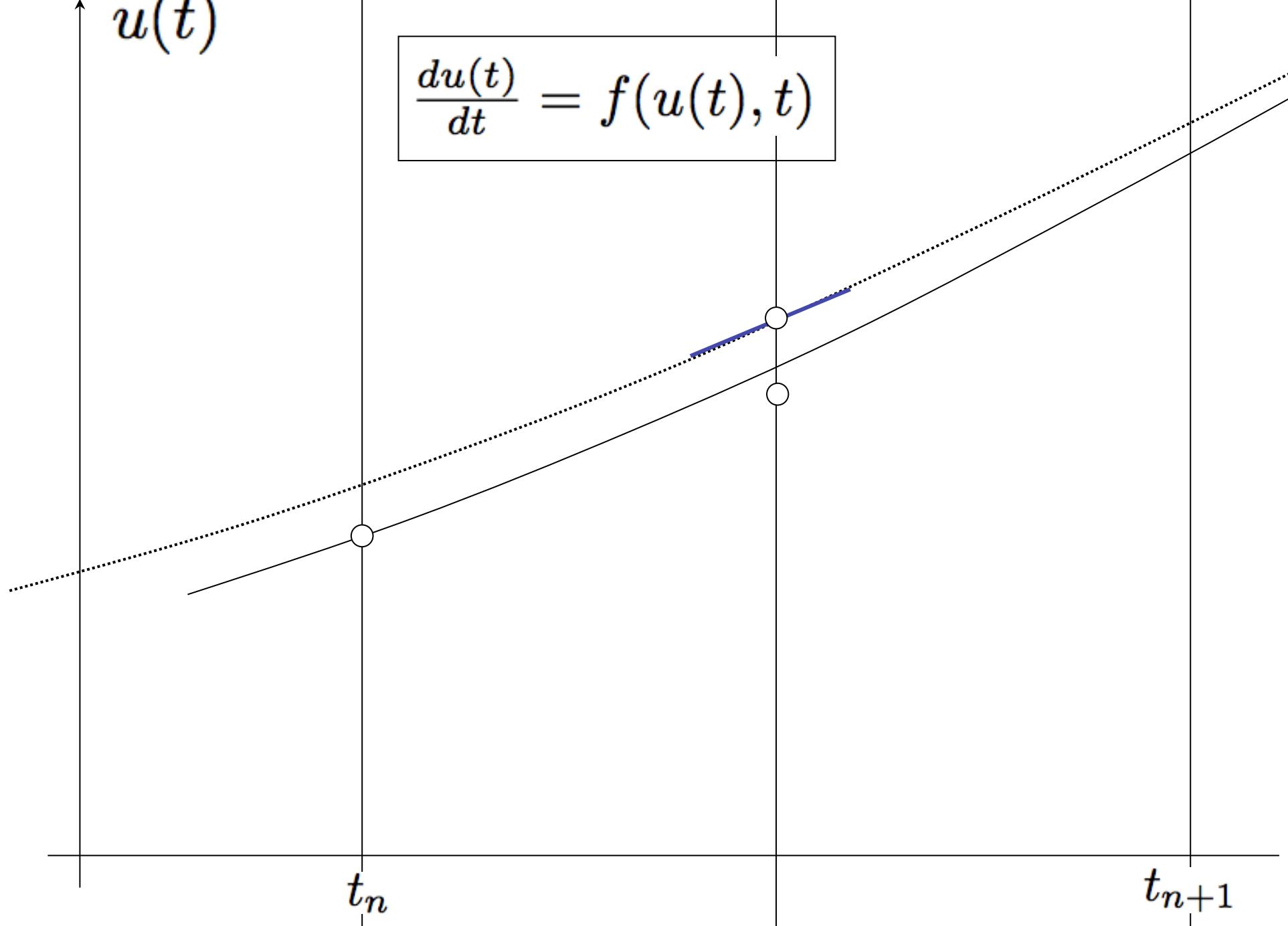






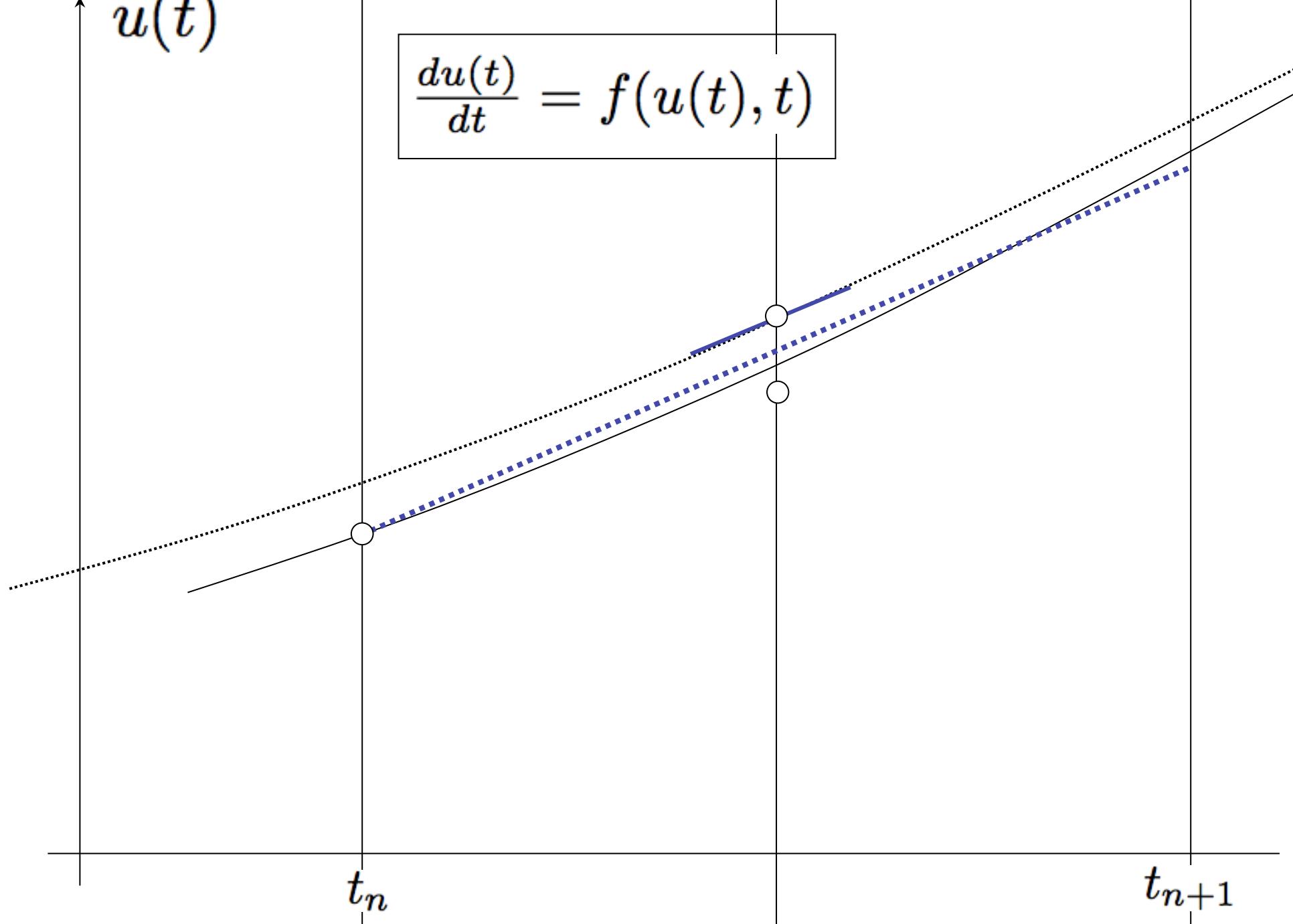
$u(t)$

$$\frac{du(t)}{dt} = f(u(t), t)$$



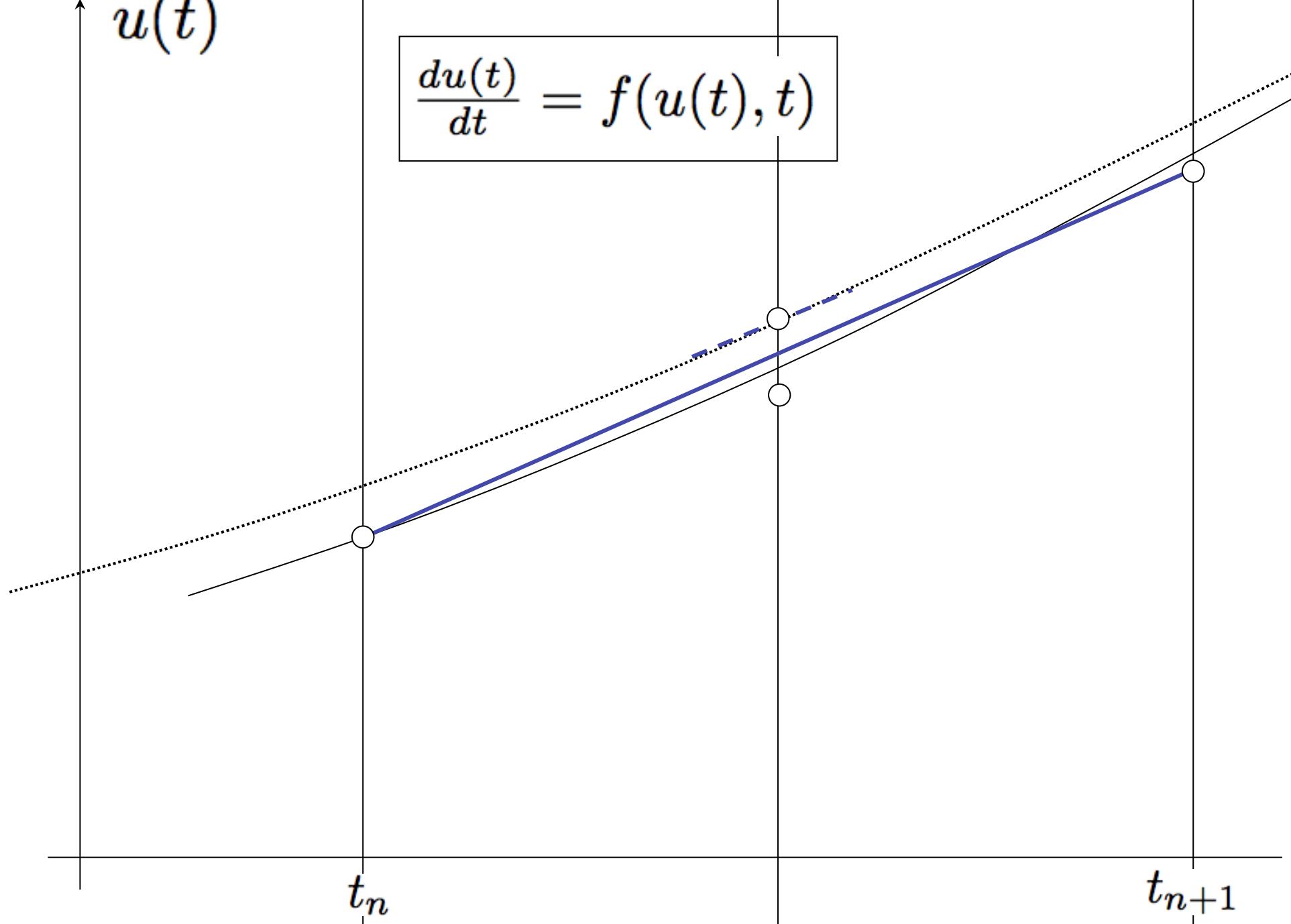
$u(t)$

$$\frac{du(t)}{dt} = f(u(t), t)$$



$u(t)$

$$\frac{du(t)}{dt} = f(u(t), t)$$

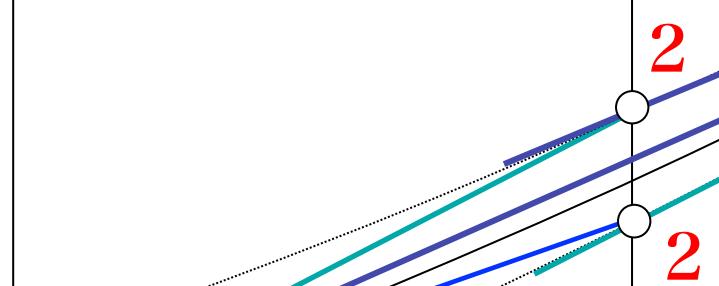


$u(t)$

$$\frac{du(t)}{dt} = f(u(t), t)$$

t_n

t_{n+1}



4-step 4th-order Runge-Kutta Integration Method

$$\frac{du(t)}{dt} = f(t, u(t))$$

$$t_0 = t_n$$

$$u_0 = u(t_0)$$

$$\underline{df_1 = \Delta t f(t_0, u_0)}$$

$$t_2 = t_0 + 0.5 \Delta t$$

$$u_2 = u_0 + 0.5 df_2$$

$$\underline{df_3 = \Delta t f(t_2, u_2)}$$

$$t_1 = t_0 + 0.5 \Delta t$$

$$u_1 = u_0 + 0.5 df_1$$

$$\underline{df_2 = \Delta t f(t_1, u_1)}$$

$$t_3 = t_0 + \Delta t$$

$$u_3 = u_0 + df_3$$

$$\underline{df_4 = f(t_3, u_3)}$$

$$u_{n+1} = u_n + \frac{1}{6}(df_1 + 2 df_2 + 2 df_3 + df_4)$$

Error $O(\Delta x^5)$ for one step, $O(\Delta x^4)$ in total.

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2}$$

$$u_0 = e^{ikx_j} \quad \text{A test wave}$$

$$\begin{aligned}
 df_1 &= \frac{\kappa \Delta t}{(\Delta x)^2} \left\{ e^{ik(x_j + \Delta x)} - 2e^{ikx_j} + e^{ik(x_j - \Delta x)} \right\} \\
 &= -\frac{2\kappa \Delta t}{(\Delta x)^2} (1 - \cos k\Delta x) e^{ikx_j} \\
 &= -\alpha e^{ikx_j} \qquad \qquad \alpha = \frac{2\kappa \Delta t}{(\Delta x)^2} (1 - \cos k\Delta x)
 \end{aligned}$$

$$u_1 = u_0 + 0.5 df_1$$

$$= \left(1 - \frac{\alpha}{2}\right) e^{ikx_j}$$

$$\begin{aligned}
 df_2 &= -\frac{2\kappa \Delta t}{(\Delta x)^2} \left(1 - \frac{\alpha}{2}\right) (1 - \cos k\Delta x) e^{ikx_j} \\
 &= -\alpha \left(1 - \frac{\alpha}{2}\right) e^{ikx_j}
 \end{aligned}$$

$$u_3 = u_0 + 0.5 \, df_2 \\ = \left(1 - \frac{\alpha}{2} + \frac{\alpha^2}{4} \right) e^{ikx_j}$$

$$df_3 = - \left(\alpha - \frac{\alpha^2}{2} + \frac{\alpha^3}{4} \right) e^{ikx_j}$$

$$u_4 = u_0 + df_3 \\ = \left(1 - \alpha + \frac{\alpha^2}{2} - \frac{\alpha^3}{4} \right) e^{ikx_j}$$

$$df_4 = - \left(\alpha - \alpha^2 + \frac{\alpha^3}{2} - \frac{\alpha^4}{4} \right) e^{ikx_j}$$

$$u_{\text{new}} = u_0 + \frac{1}{6} (df_1 + 2 \, df_2 + 2 \, df_3 + df_4) \\ = \left(1 - \alpha + \frac{\alpha^2}{2} - \frac{\alpha^3}{6} + \frac{\alpha^4}{24} \right) e^{ikx_j} \\ = \left\{ 1 + \frac{(-\alpha)}{1!} + \frac{(-\alpha)^2}{2!} + \frac{(-\alpha)^3}{3!} + \frac{(-\alpha)^4}{4!} \right\} e^{ikx_j}$$

By one step integration of 4-th order Runge-Kutta method,

$$u_{\text{new}} = \left\{ 1 + \frac{(-\alpha)}{1!} + \frac{(-\alpha)^2}{2!} + \frac{(-\alpha)^3}{3!} + \frac{(-\alpha)^4}{4!} \right\} e^{ikx_j}$$

$$\alpha = \frac{2\kappa\Delta t}{(\Delta x)^2} (1 - \cos k\Delta x)$$

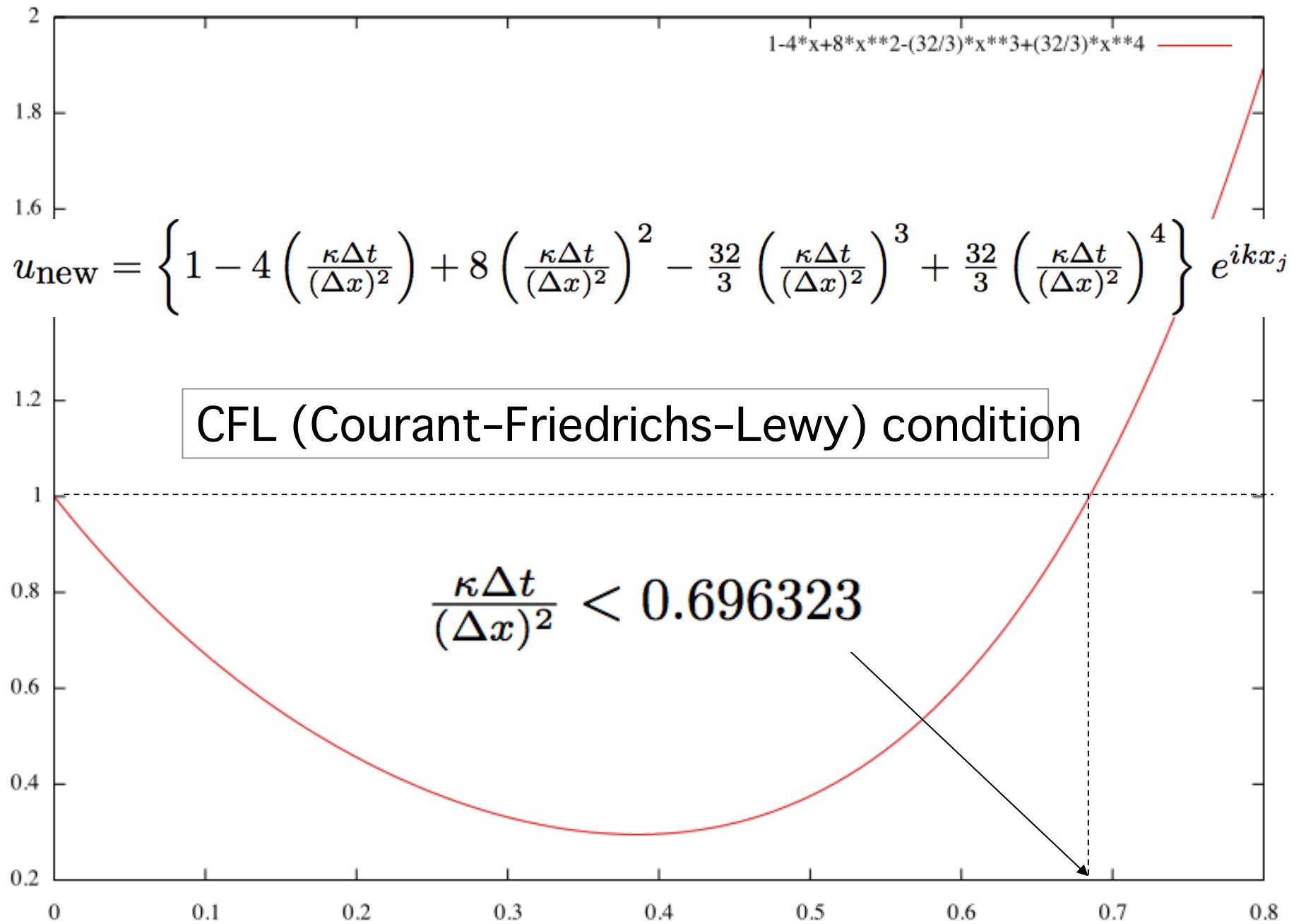
When $k\Delta x \ll 1$ $\alpha \sim \frac{\kappa\Delta t}{(\Delta x)^2} (k\Delta x)^2 = k^2 \kappa \Delta t$

$$u_{\text{exact}} = e^{-k^2 \kappa \Delta t} e^{ikx_j} = e^{-\alpha \Delta t}$$

$$\text{Error in 1step} = O[(\Delta t)^5] \implies \text{Error in total} = O[(\Delta t)^4]$$

When $k\Delta x = \pi$, $\alpha = \frac{4\kappa\Delta t}{(\Delta x)^2}$

$$u_{\text{new}} = \left\{ 1 - 4 \left(\frac{\kappa\Delta t}{(\Delta x)^2} \right) + 8 \left(\frac{\kappa\Delta t}{(\Delta x)^2} \right)^2 - \frac{32}{3} \left(\frac{\kappa\Delta t}{(\Delta x)^2} \right)^3 + \frac{32}{3} \left(\frac{\kappa\Delta t}{(\Delta x)^2} \right)^4 \right\} e^{ikx_j}$$



Simple Numerical Simulation with Fortran90 Code

$$\boxed{\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}}$$

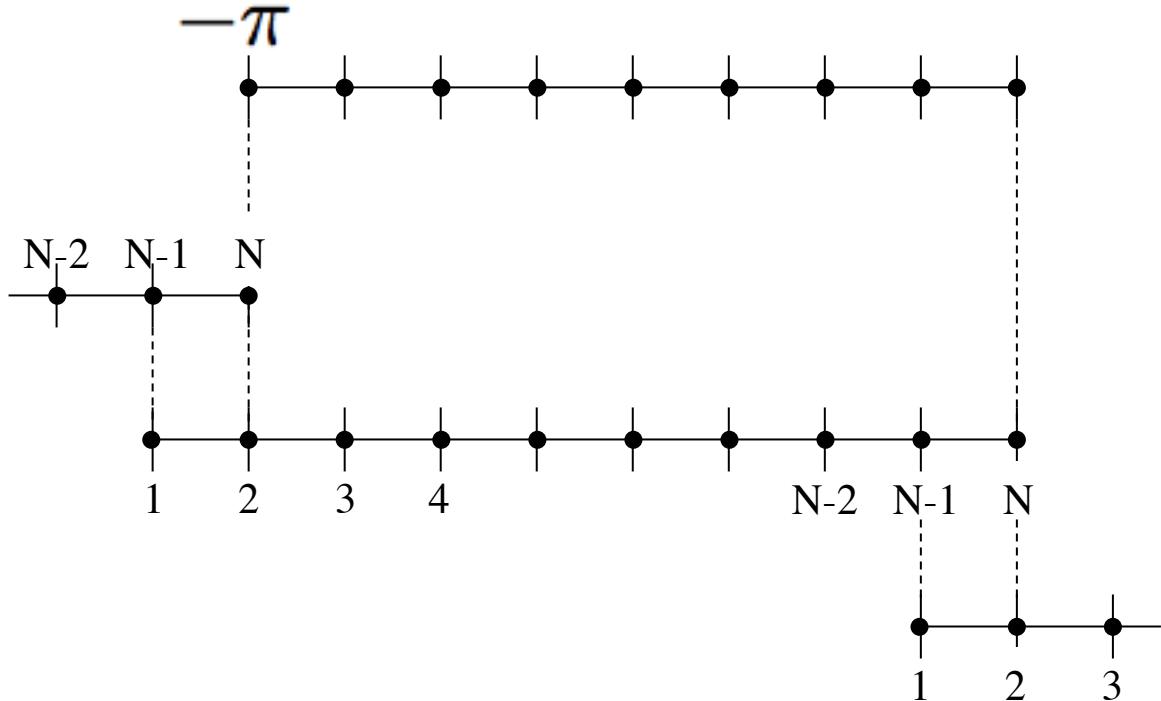
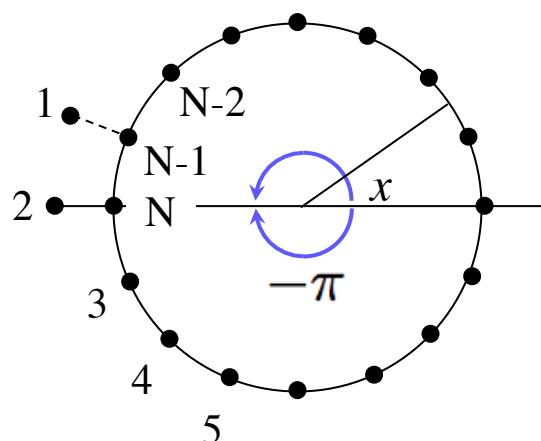
A Sample Code in FDM

$$\frac{d\psi_j}{dt} = \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}$$

$$\frac{d\psi_j}{dt} = f(\psi_1, \psi_2, \dots, \psi_N)$$

==> 4-step (4th order) Runge-Kutta method

Periodic boundary condition



```
subroutine iBoundary_condition(psi)
    real(DP), dimension(nx), intent(inout) :: psi

    psi(1)      = psi(nx-1)
    psi(nx)     = psi(2)

end subroutine iBoundary_condition
```

Now let's see the code: main.f90

```
do nloop = 1 , nloop_max

    dpsio1(:) = rk4_step('1st',dt,dx,psi)
    call iBoundary_condition(dpsio1)

    dpsio2(:) = rk4_step('2nd',dt,dx,psi,dpsio1)
    call iBoundary_condition(dpsio2)

    dpsio3(:) = rk4_step('3rd',dt,dx,psi,dpsio2)
    call iBoundary_condition(dpsio3)

    dpsio4(:) = rk4_step('4th',dt,dx,psi,dpsio3)
    call iBoundary_condition(dpsio4)

    time = time + dt
    psi(:) = psi(:) + ONE_SIXTH*(dpsio1(:)) &
              +2*dpsio2(:) &
              +2*dpsio3(:) &
              +dpsio4(:))

end do
```

Runge-Kutta step (rk.f90)

```
function rk4__step(nth,dt,dx,psi,dpsi_prev)      &
                           result(dpsi_new)

character(len=3), intent(in)                      :: nth
real(DP), intent(in)                            :: dt
real(DP), intent(in)                            :: dx
real(DP), dimension(:), intent(in)    :: psi
real(DP), dimension(size(psi,dim=1)),   &
                           intent(in), optional :: dpsi_prev
real(DP), dimension(size(psi,dim=1)) :: dpsi_new
real(DP), dimension(size(psi,dim=1)) :: psi_
```

```
select case (nth)
case ('1st')
    dpsi_new(:) = dt*diffusion_equation(size(psi,dim=1), &
                                         dx,psi)
case ('2nd')
    psi_(:) = psi(:) + dpsi_prev(:)*0.5_DP
    dpsi_new(:) = dt*diffusion_equation(size(psi,dim=1), &
                                         dx,psi_)
case ('3rd')
    psi_(:) = psi(:) + dpsi_prev(:)*0.5_DP
    dpsi_new(:) = dt*diffusion_equation(size(psi,dim=1), &
                                         dx,psi_)
case ('4th')
    psi_(:) = psi(:) + dpsi_prev(:)
    dpsi_new(:) = dt*diffusion_equation(size(psi,dim=1), &
                                         dx,psi_)
end select

end function rk4_step
```

diffusion_equation (rk.f90)

```
function diffusion_equation(nx,dx,psi)
    integer, intent(in)                      :: nx
    real(DP), intent(in)                      :: dx
    real(DP), dimension(nx), intent(in) :: psi
    real(DP), dimension(nx)                  :: diffusion_equation

    integer :: i
    real(DP) :: dx2

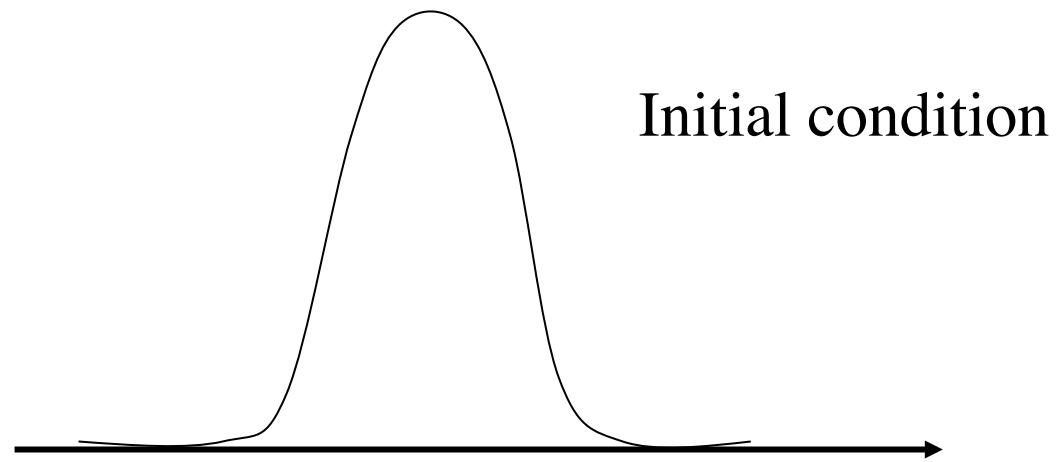
    dx2 = namelist__double('Diffusion_coeff')/(dx**2)

    do i = 2 , nx-1
        diffusion_equation(i) = dx2*(psi(i+1)-2*psi(i)+psi(i-1))
    end do

end function diffusion_equation
```

$$\kappa \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}$$

Let's run the code



src/DiffusionEquation

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2}$$

Time Integration in Fourier Spectral Method

$$\frac{d\psi_m(t)}{dt} = -m^2 \psi_m(t)$$

$$\psi_m(t) = \psi_m(0) \exp(-m^2 t)$$

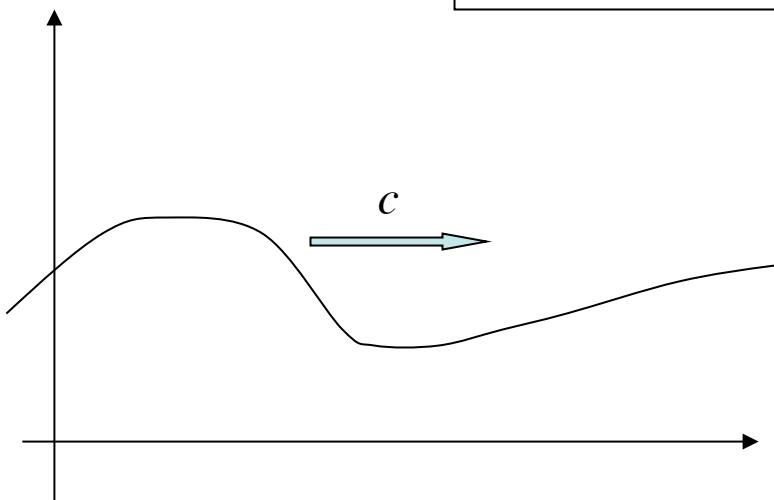
$$\implies \psi(x, t) = \sum_m \psi_m(0) \frac{\exp(imx - m^2 t)}{\sqrt{2\pi}}$$

This is an exceptionally lucky case, it's not always that simple, especially...

Nonlinear terms in spectral methods

Burgers' equation

$$\frac{\partial \psi}{\partial t} = -\psi \frac{\partial \psi}{\partial x} + \nu \frac{\partial^2 \psi}{\partial x^2}$$



$$\frac{\partial \psi}{\partial t} = -c \frac{\partial \psi}{\partial x}$$

Solution:

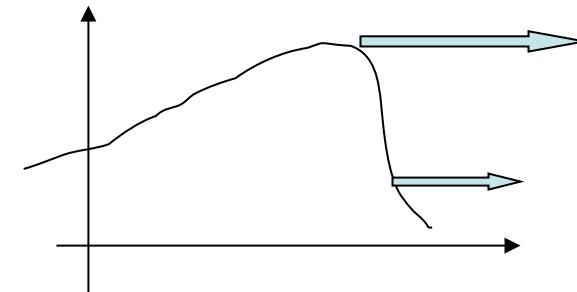
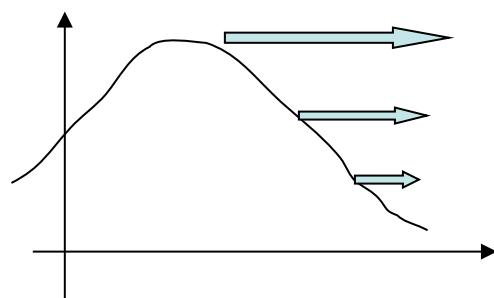
$$\psi(x, t) = f(x - ct)$$

Burgers' equation

$$\frac{\partial \psi}{\partial t} = -\psi \frac{\partial \psi}{\partial x} + \nu \frac{\partial^2 \psi}{\partial x^2}$$

Diffusion term

$$\frac{\partial \psi}{\partial t} = -\psi \frac{\partial \psi}{\partial x}$$



To solve Burgers' equation by spectral methods

$$\psi(x, t) = \sum_k \psi_k(t) \frac{\exp(ikx)}{\sqrt{2\pi}}$$

$$\frac{\partial \psi}{\partial t} = -\psi \frac{\partial \psi}{\partial x} + \nu \frac{\partial^2 \psi}{\partial x^2}$$

$$\rightarrow \quad \frac{d\psi_m(t)}{dt} = - \sum_k \frac{\psi_k(t)\psi_{m-k}(t)}{\sqrt{2\pi}} - \nu m^2 \psi_m(t)$$

convolution

To solve Burgers' equation by Spectral Methods

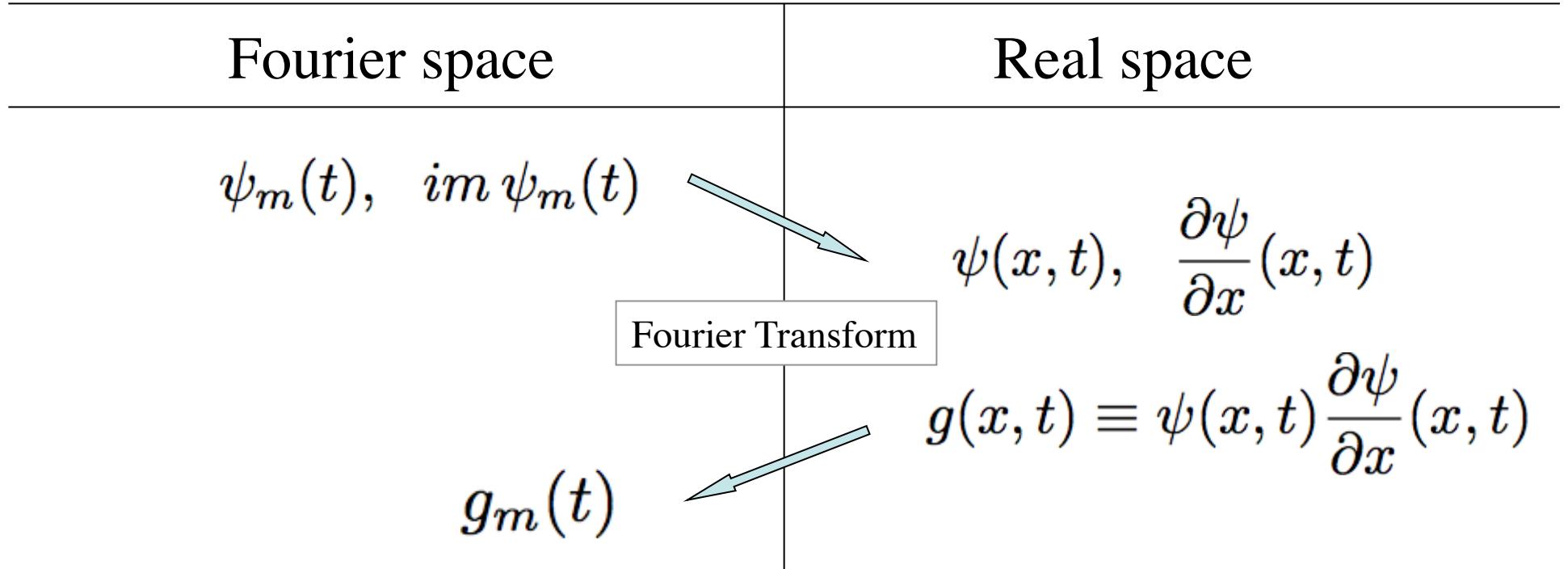
$$\left\{ \begin{array}{l} \frac{d\psi_m(t)}{dt} = - \sum_k \underbrace{\frac{\psi_k(t)\psi_{m-k}(t)}{\sqrt{2\pi}}}_{M \text{ multiplications}} - \nu m^2 \psi_m(t) \\ \vdots \end{array} \right.$$

M set of equations

$O(M^2)$ calculations

Pseudo-spectral Method

$$\frac{\partial \psi}{\partial t} = -\psi \frac{\partial \psi}{\partial x} + \nu \frac{\partial^2 \psi}{\partial x^2}$$



$$\frac{d\psi_m}{dt} = -g_m(t) - m^2 \psi_m(t)$$

Fast Fourier Transform (FFT)

Fourier space	Real space
f_m	$f_j(x) = \sum_m f_m \frac{\exp(imx)}{\sqrt{2\pi}}$
$f_m = \int_{-\pi}^{\pi} f_j(x) \frac{\exp(-imx)}{\sqrt{2\pi}} dx$	$f_j(x)$

$O(M \log M)$ calculations

$\ll O(M^2)$

Nonlinear terms: FDM

$$\frac{\partial \psi}{\partial t} = -\psi \frac{\partial \psi}{\partial x} + \nu \frac{\partial^2 \psi}{\partial x^2}$$

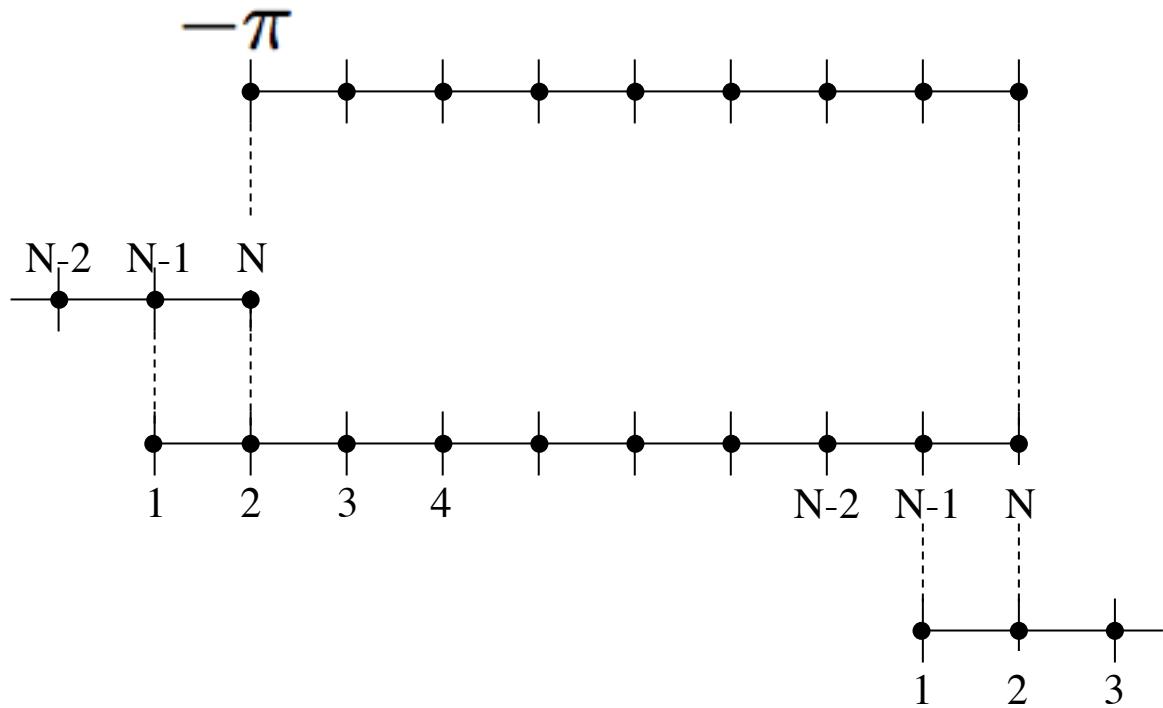
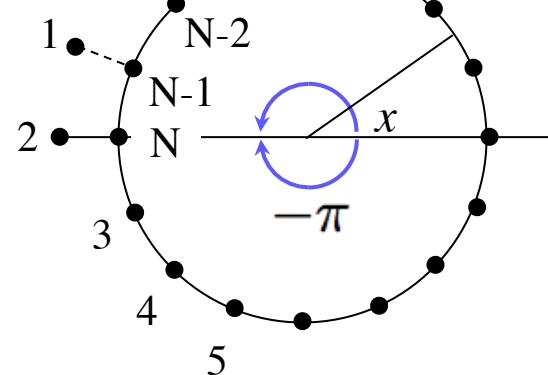
$$\rightarrow \quad \frac{d\psi_j}{dt} = -\psi_j \frac{\psi_{j+1} - \psi_{j-1}}{2\Delta x} + \nu \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}$$

Let's see the code.

code

- src/BurgersEquation

Burgers' equation by FDM



$$\frac{d\psi_j}{dt} = -\psi_j \frac{\psi_{j+1} - \psi_{j-1}}{2\Delta x} + \nu \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}$$

Runge-Kutta 1st step (rk4.f90)

```
function rk4_1st(dt,dx,psi) result(dpsi01)
    real(DP), intent(in)          :: dt
    real(DP), intent(in)          :: dx
    real(DP), dimension(:), intent(in)  :: psi
    real(DP), dimension(size(psi,dim=1)) :: dpsi01

    real(DP), dimension(size(psi,dim=1)) :: psi_
    dpsi01(:) = dt*burgers_equation(size(psi,dim=1),dx,psi)

end function rk4_1st
```

burgers_equation (rk4.f90)

```
function burgers_equation(nx,dx,psi)
    integer, intent(in)                      :: nx
    real(DP), intent(in)                     :: dx
    real(DP), dimension(nx), intent(in) :: psi
    real(DP), dimension(nx)                 :: burgers_equation

    integer :: i
    real(DP) :: dx1, dx2
    
$$\frac{d\psi_j}{dt} = -\psi_j \frac{\psi_{j+1} - \psi_{j-1}}{2\Delta x} + \nu \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}$$

    dx1 = 1.0_DP / (2*dx)
    dx2 = namelist_double('Diffusion_coeff')/(dx**2)

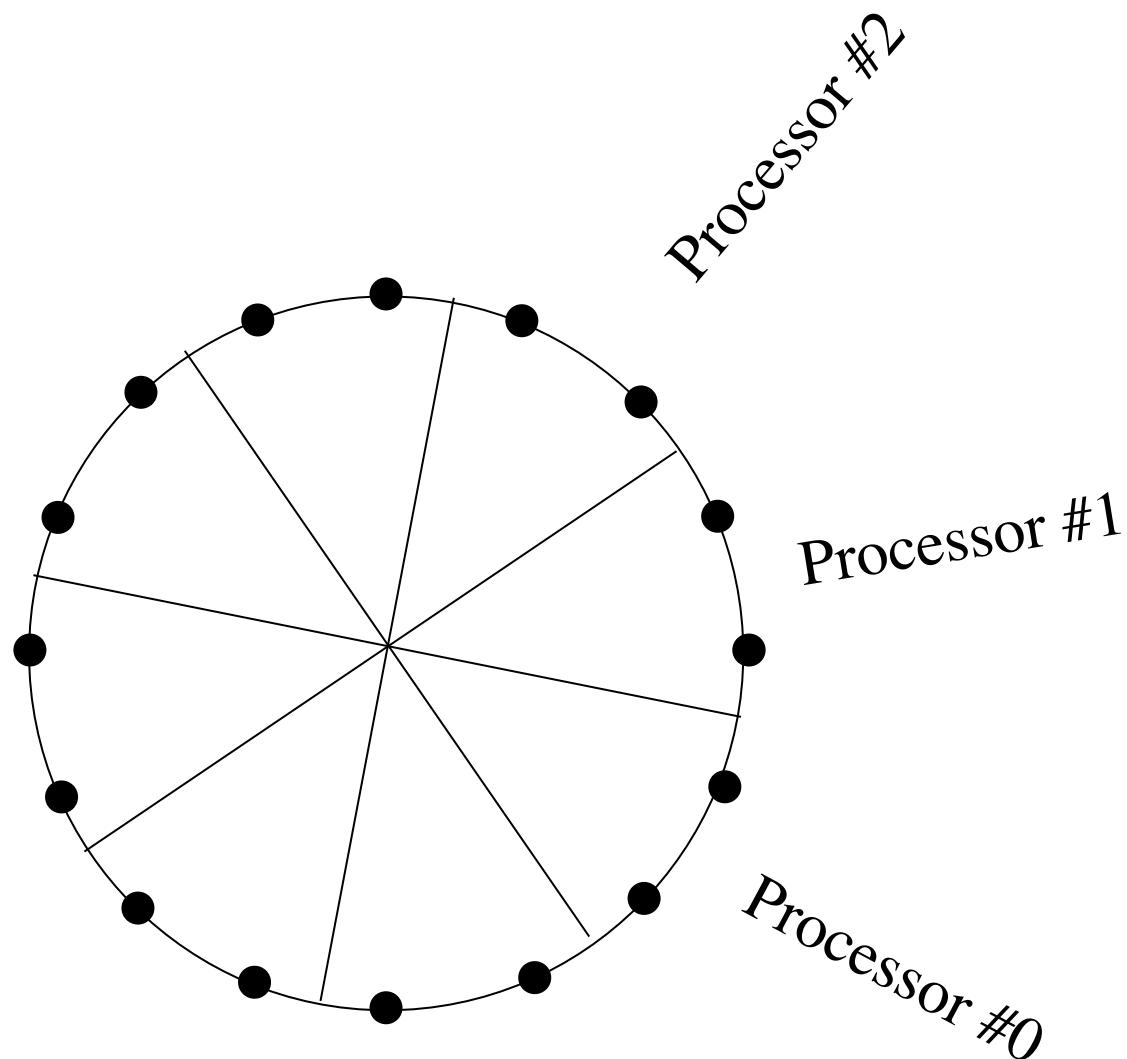
    do i = 2 , nx-1
        burgers_equation(i) = - psi(i)*dx1*(psi(i+1)-psi(i-1)) &
                               + dx2*(psi(i+1)-2*psi(i)+psi(i-1))
    end do

end function burgers_equation
```

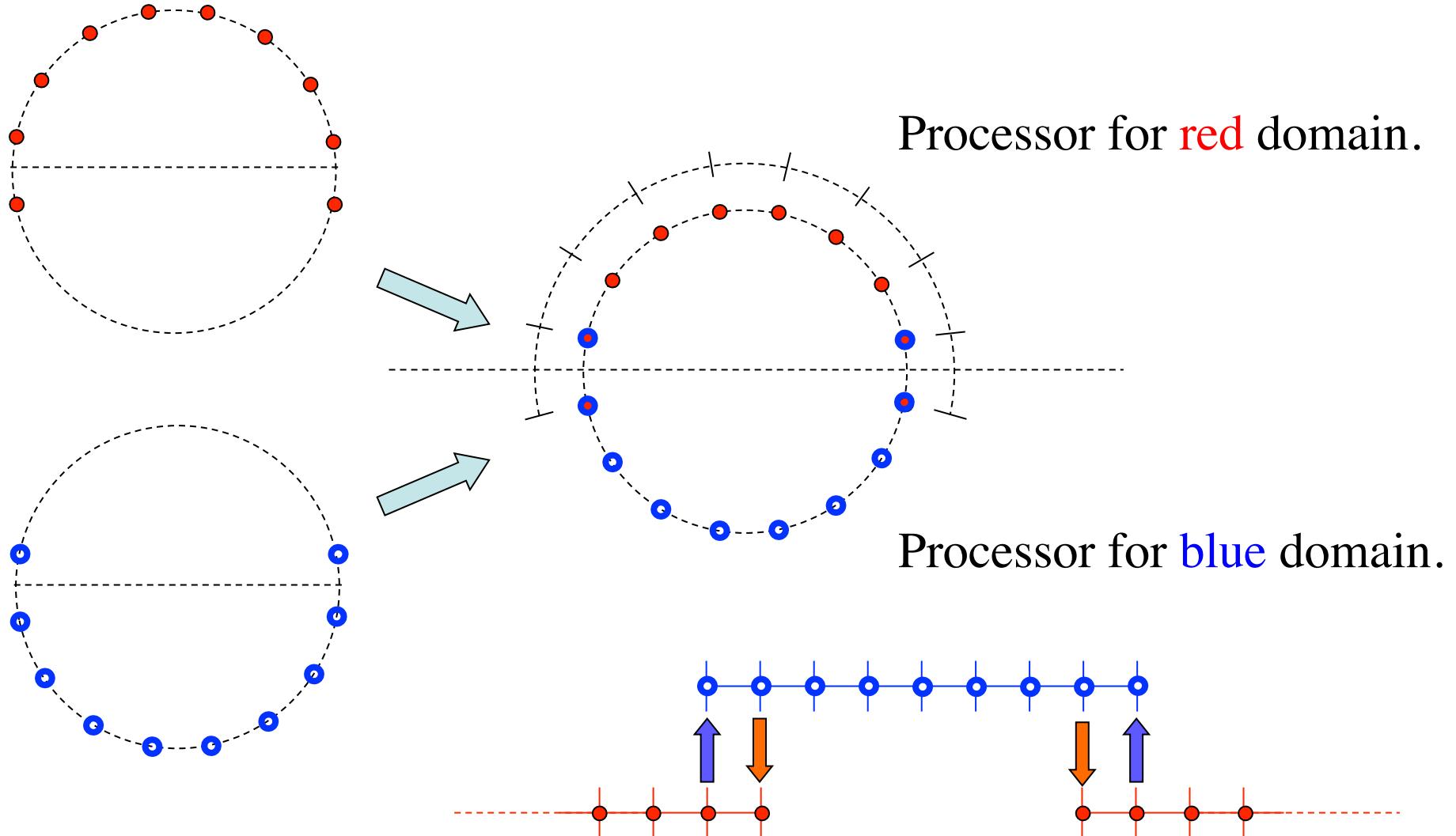
Let's run the code

src/BuergersEquation

Parallel processing by domain decomposition



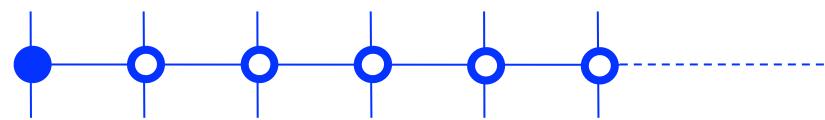
Parallel computation by 2 processors



Inter process communication

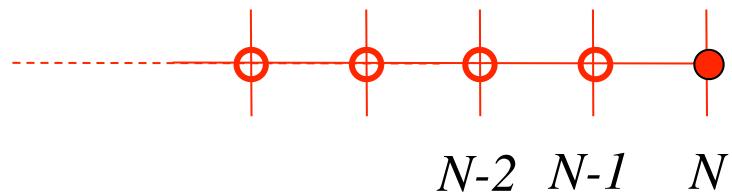
A PDE solver in
the **blue** domain

1 2 3

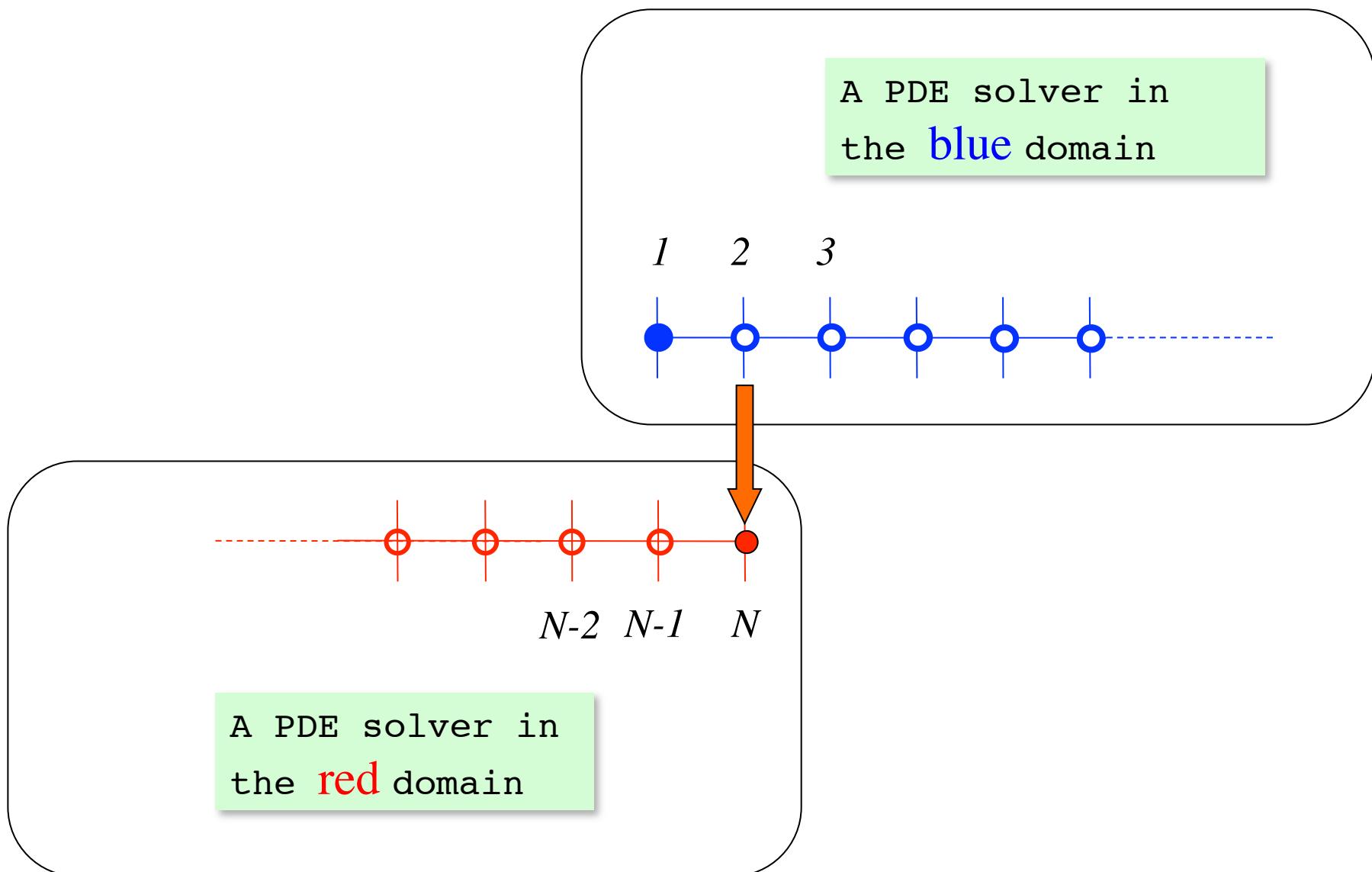


Set the boundary value
from other solver.

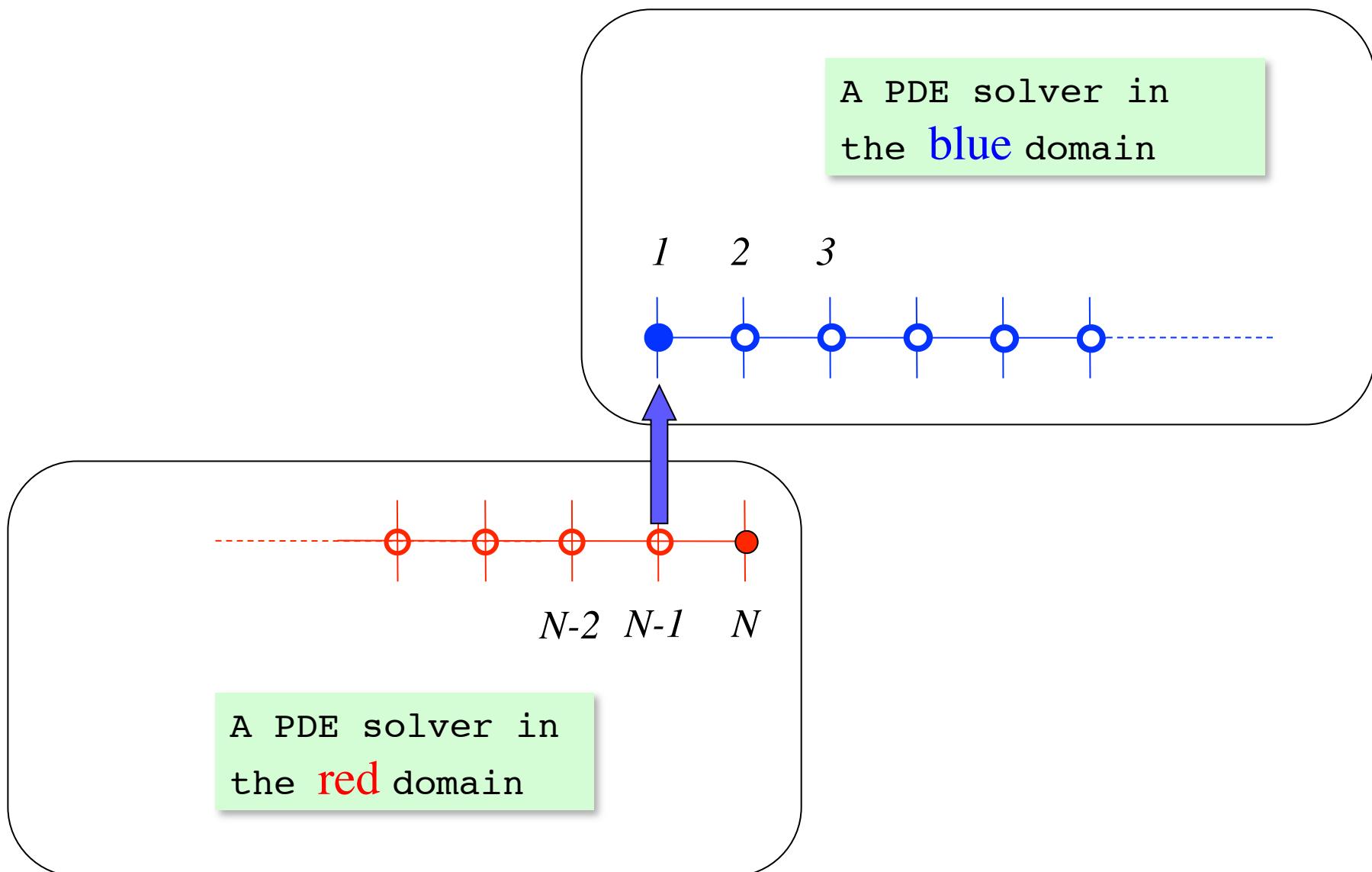
A PDE solver in
the **red** domain



Inter process communication



Inter process communication



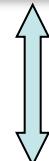
In the code

In the red processor:

```
do i = 2 , nx-1  
    diffusion_equation(i) = dx2*(psi(i+1)-2*psi(i)+psi(i-1))  
end do
```

In the blue processor:

```
do i = 2 , nx-1  
    diffusion_equation(i) = dx2*(psi(i+1)-2*psi(i)+psi(i-1))  
end do
```



Same computation, same code.

In the code

In the red processor:

```
do i = 2 , nx-1  
    diffusion_equation(i) = dx2*(psi(i+1)-2*psi(i)+psi(i-1))  
end do
```

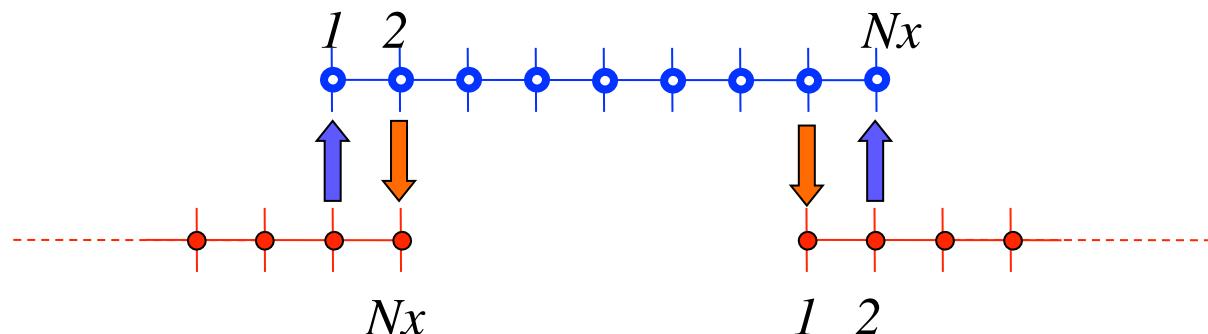
In the blue processor:

```
do i = 2 , nx-1  
    diffusion_equation(i) = dx2*(psi(i+1)-2*psi(i)+psi(i-1))  
end do
```



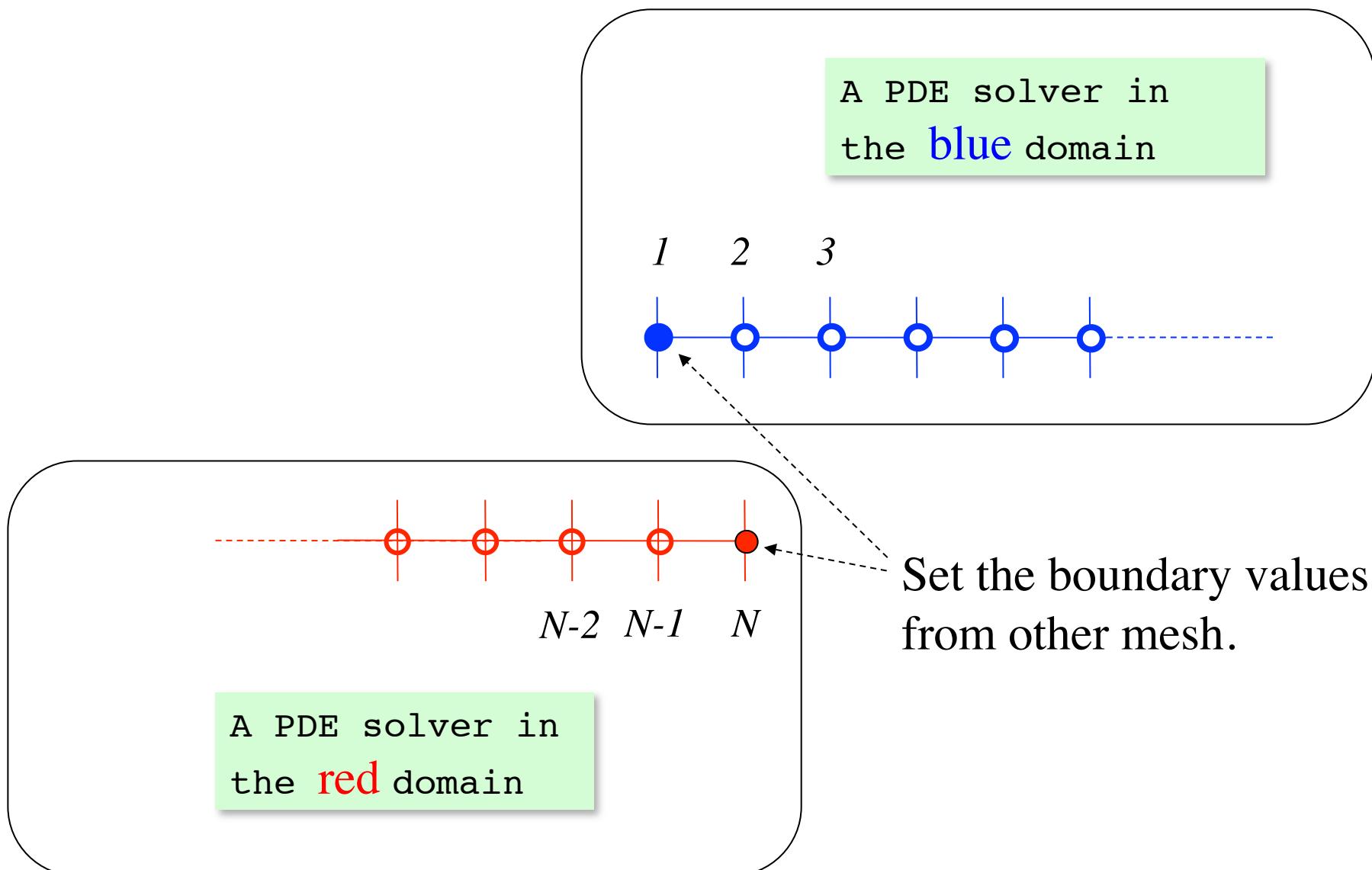
Same computation, same code.

“Boundary condition”



Inter-process communication (by MPI, etc.)

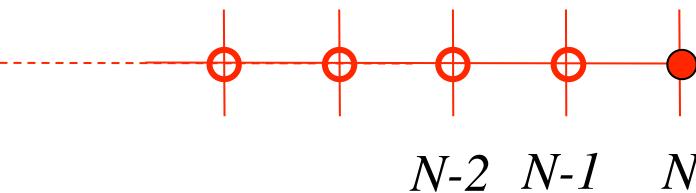
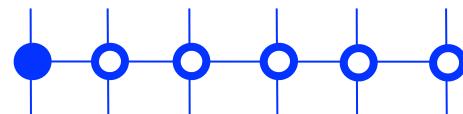
Two independent PDE solvers



Two independent PDE solvers: Grid size can be different

A PDE solver in
the **blue** domain

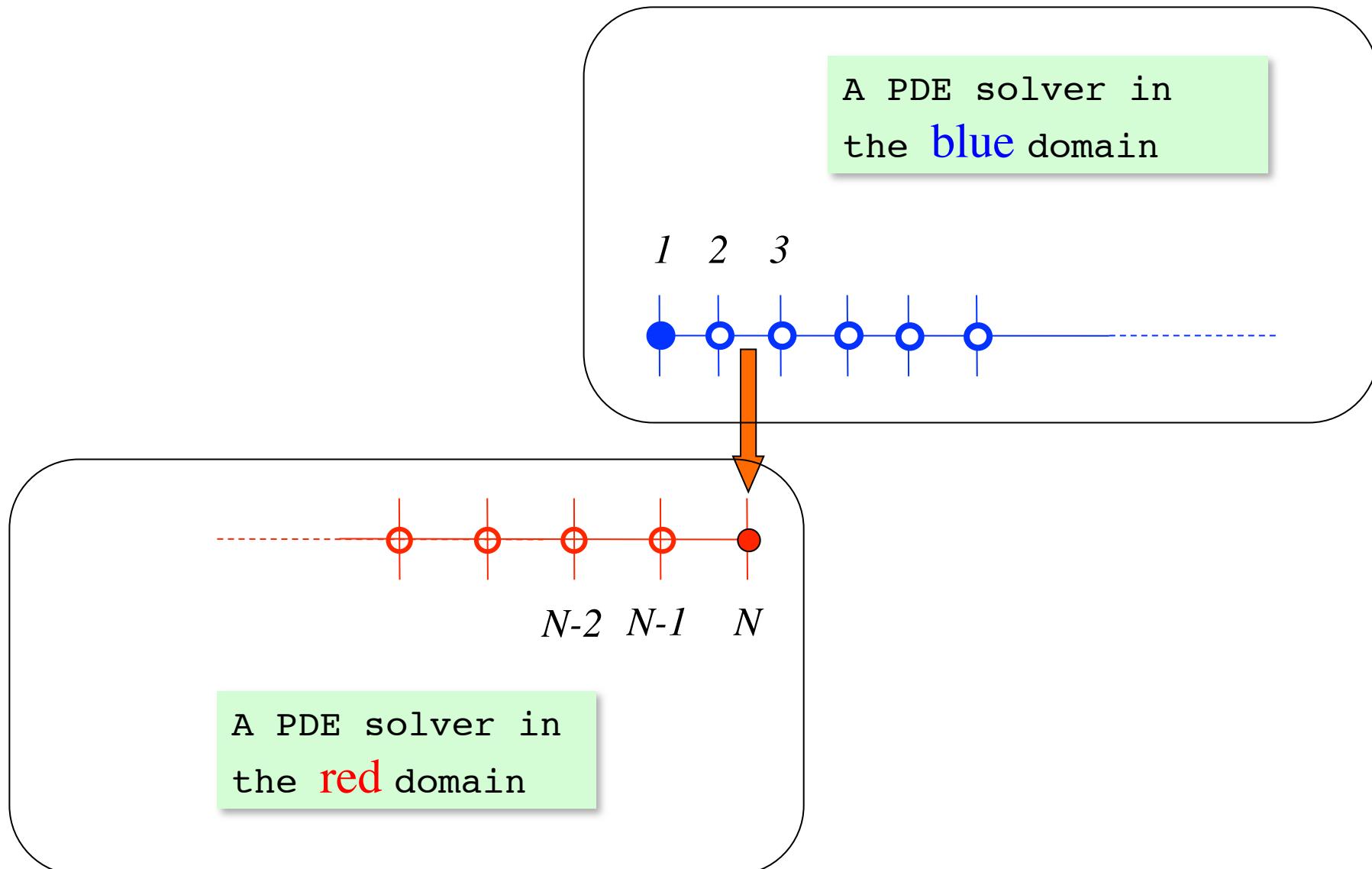
1 2 3



$N-2$ $N-1$ N

A PDE solver in
the **red** domain

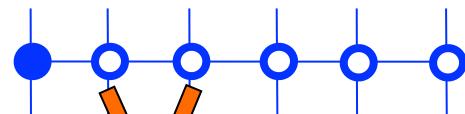
Two independent PDE solvers: Grid size can be different



No problem

A PDE solver in
the **blue** domain

1 2 3

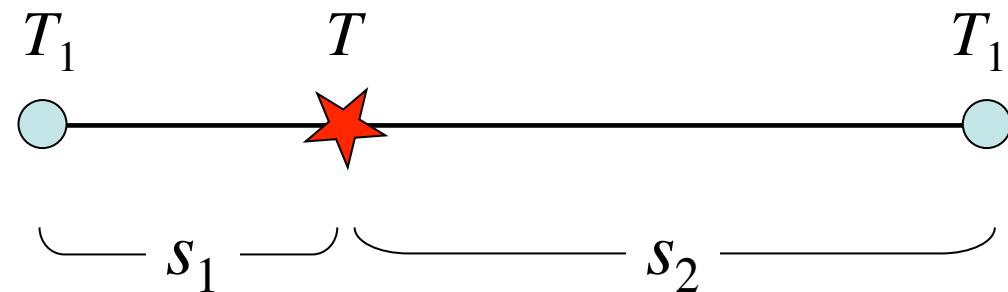


$N-2$ $N-1$ N

A PDE solver in
the **red** domain

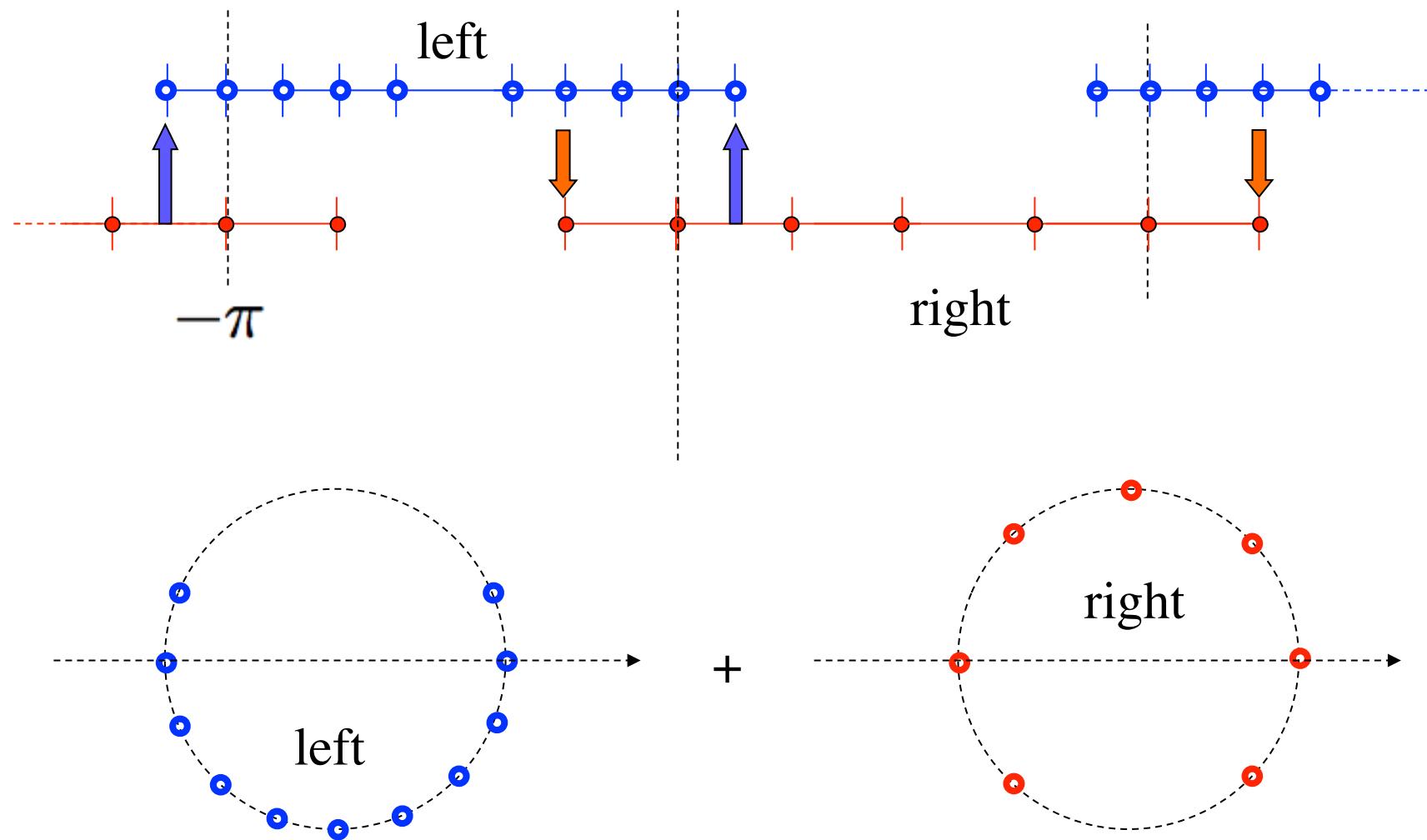
“Guess” the inter-grid value.
==> Interpolation.

Linear interpolation in 1-D



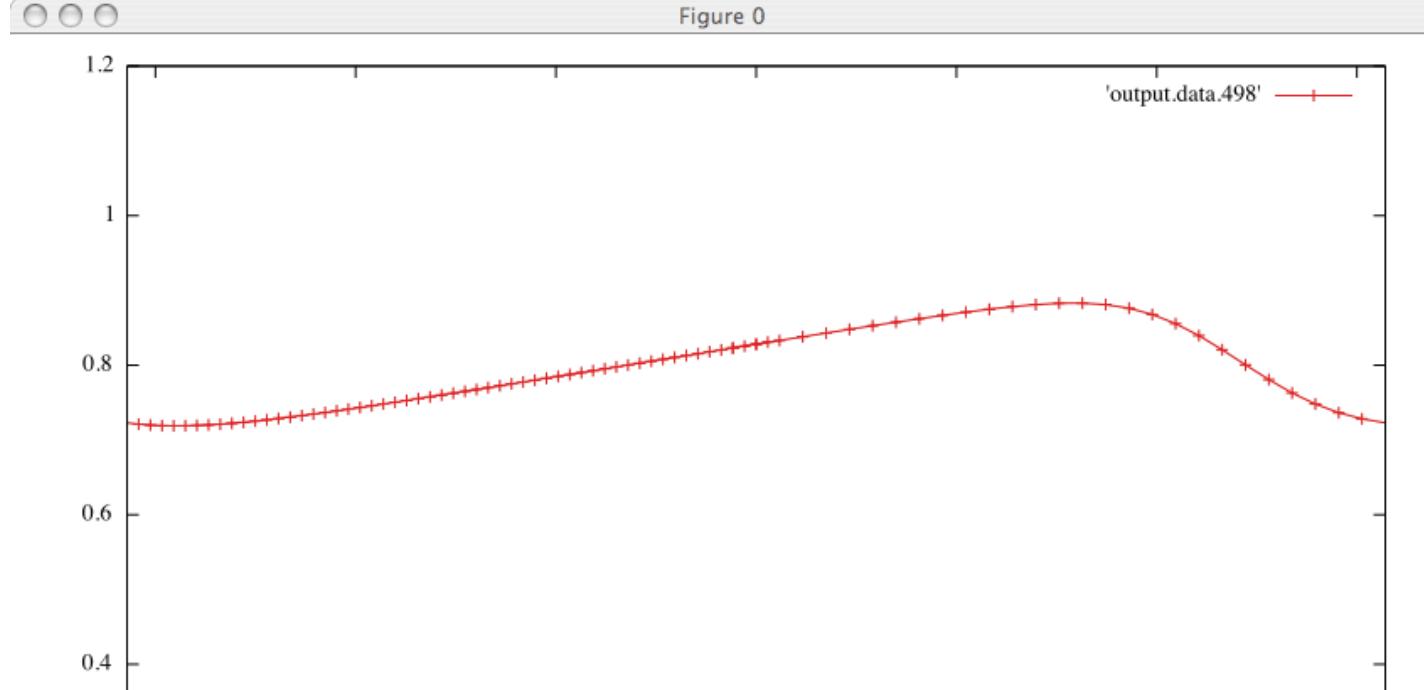
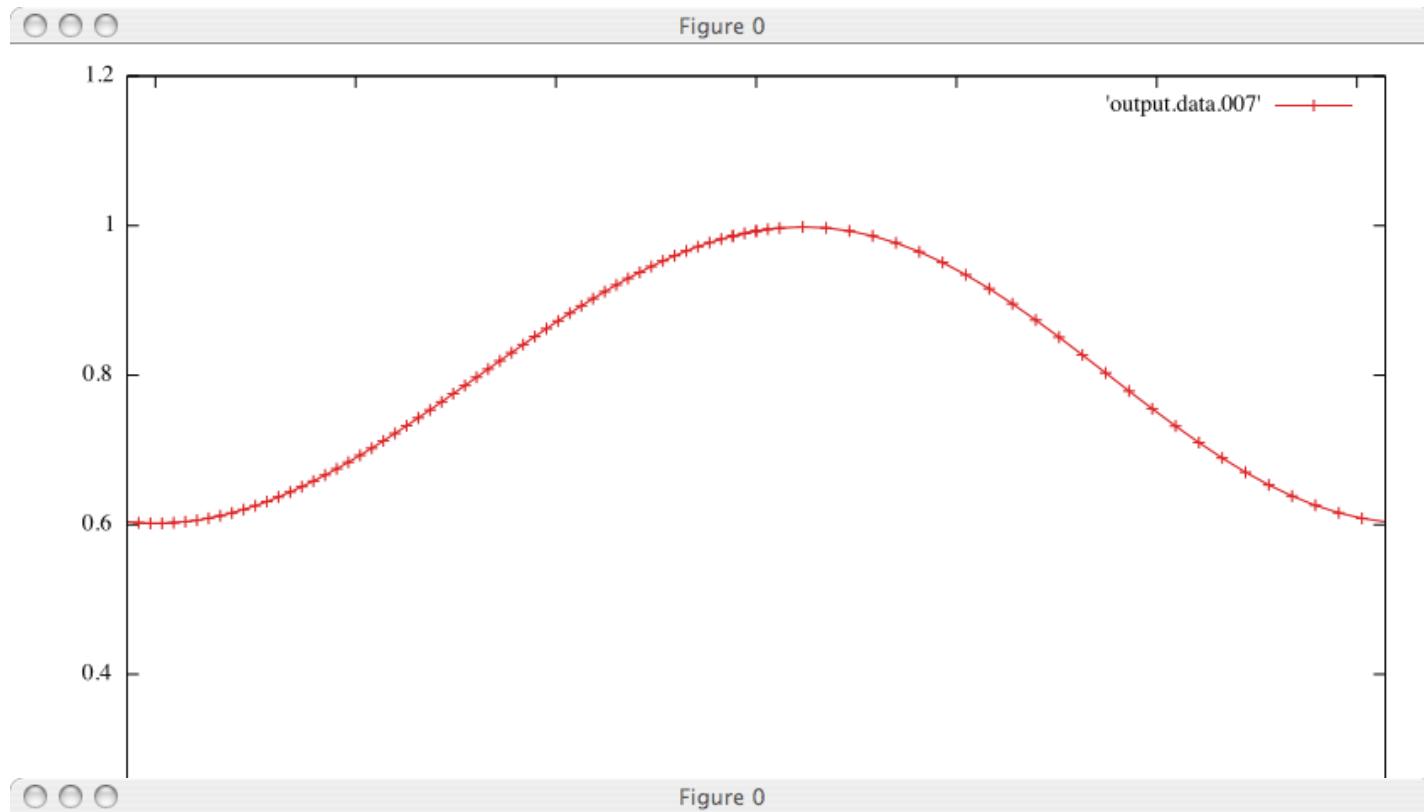
$$T = (s_2 T_1 + s_1 T_2) / (s_1 + s_2)$$

Overset grid method : 1-D Burgers' equation



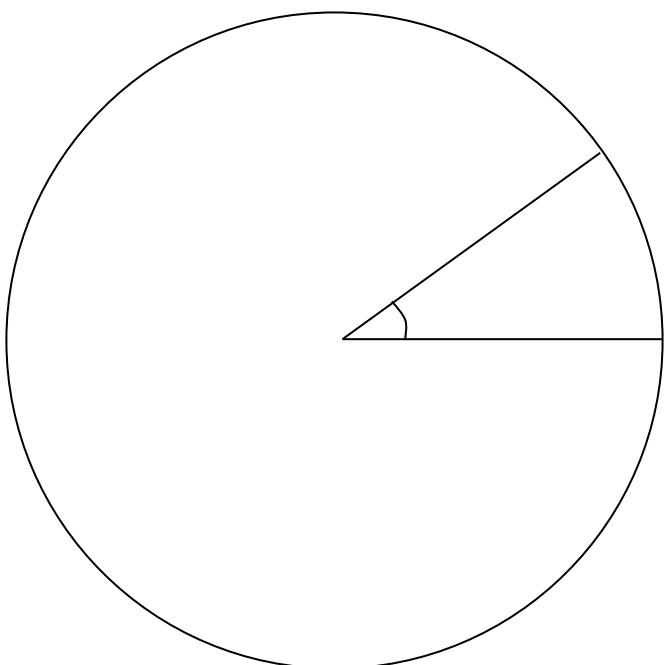
Let's run the code

Code
- src/SampleChimera

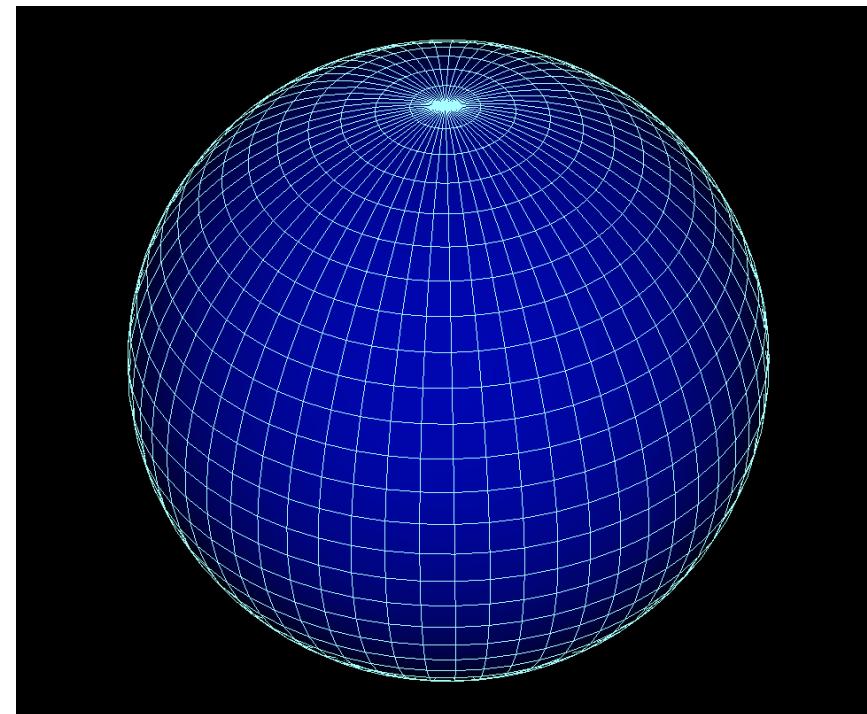


Numerical Methods on a Sphere

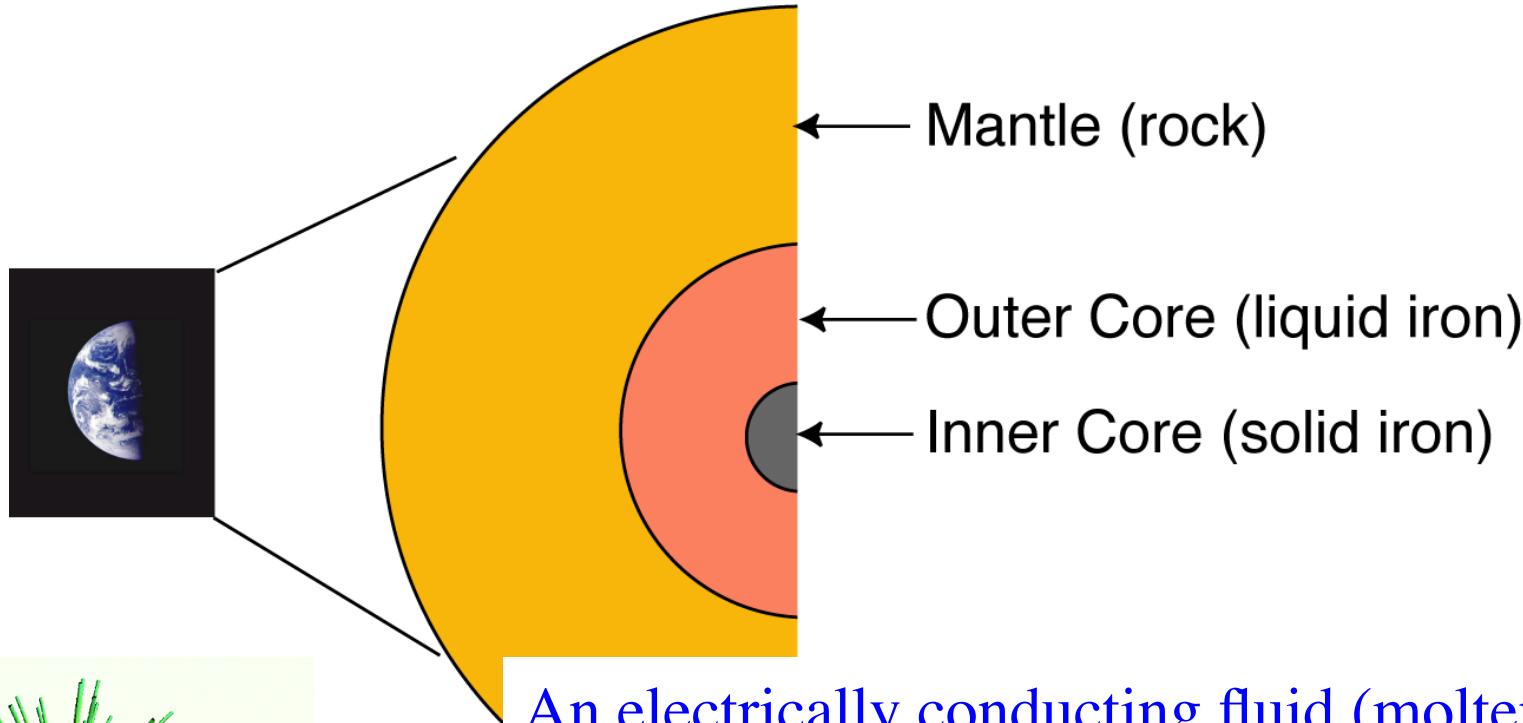
2D... circle



3D... sphere

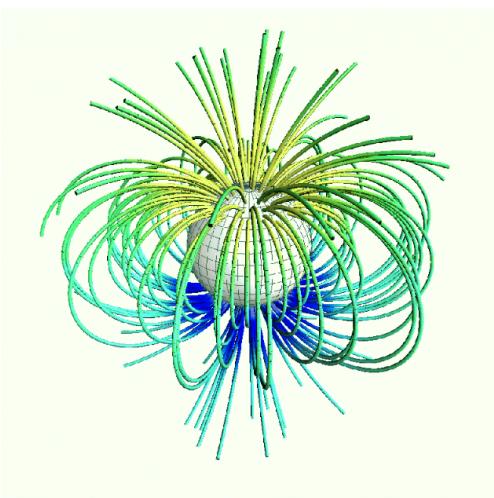


MHD Fluid in the Earth



An electrically conducting fluid (molten iron).

- MHD eqs.
- Convection
- Magnetic field (electric current) generation
- MHD dynamo



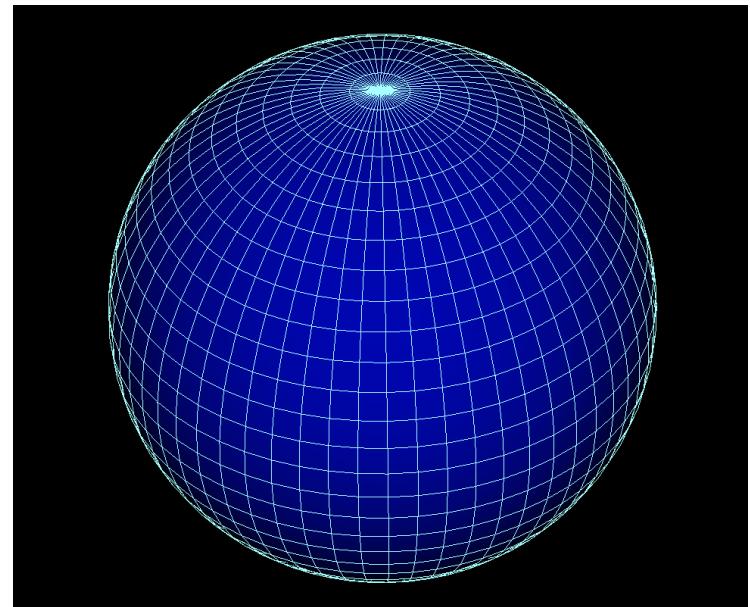
Coordinate singularity causes two different problems

1. **On** the poles:

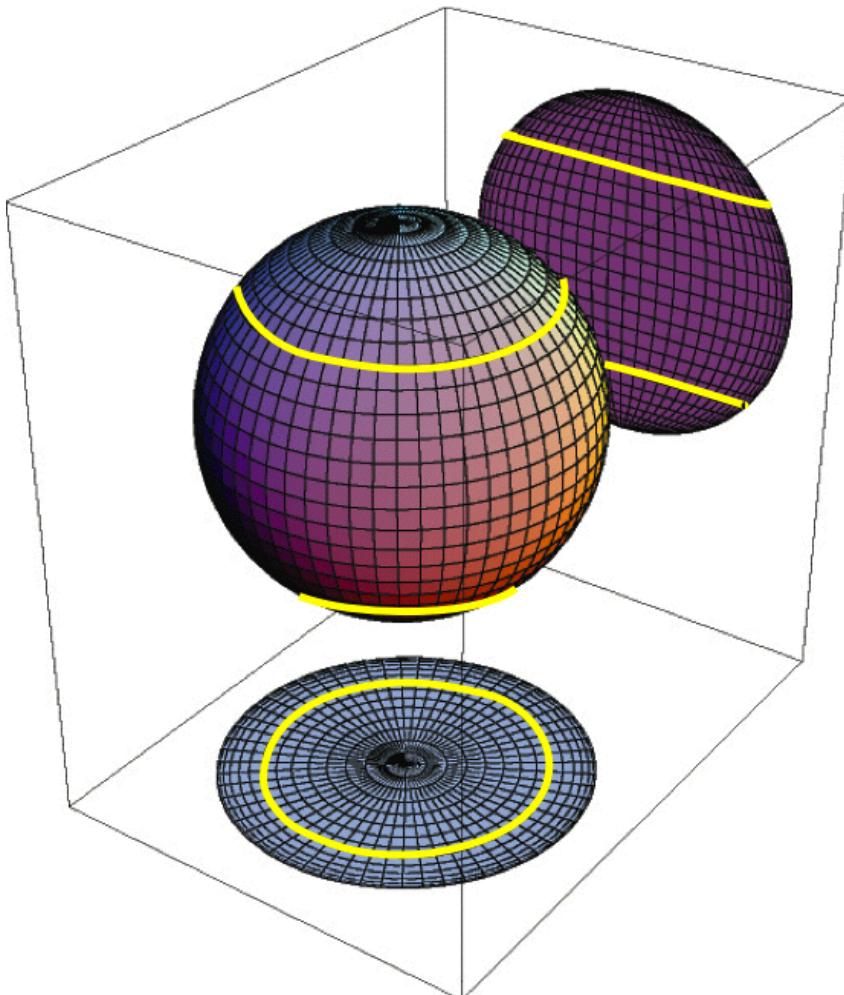
- Need's special cares;
e.g., L'Hospital's theorem.
- Not serious.

2. **Near** the poles:

- Grid convergence.
- Serious; waste of CPU time.



Grid convergence = inefficiency

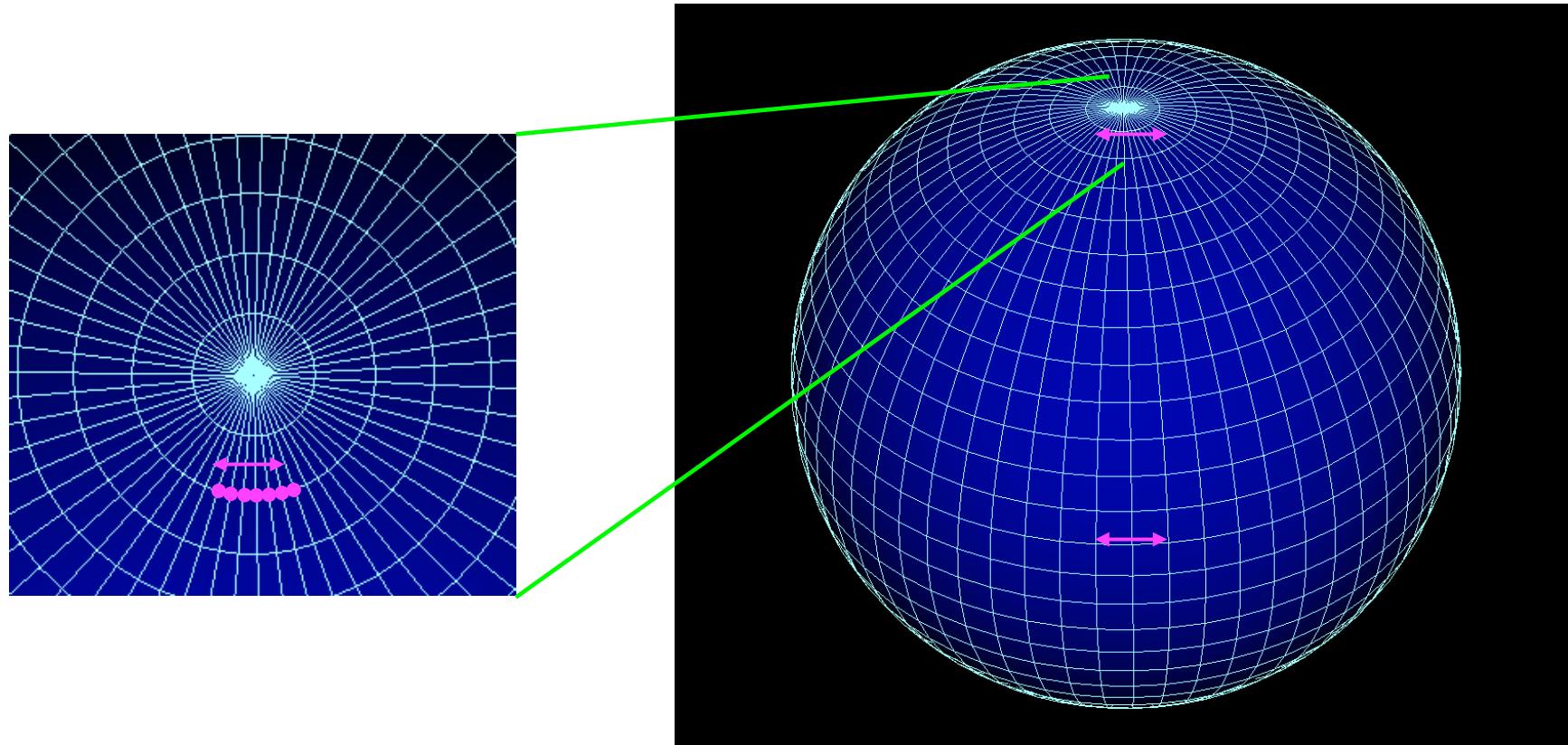


84% of grid points are located in high-latitude part ($>45^\circ$ N and S).

Low latitude part (between 45° N and S) is covered by only 16%.

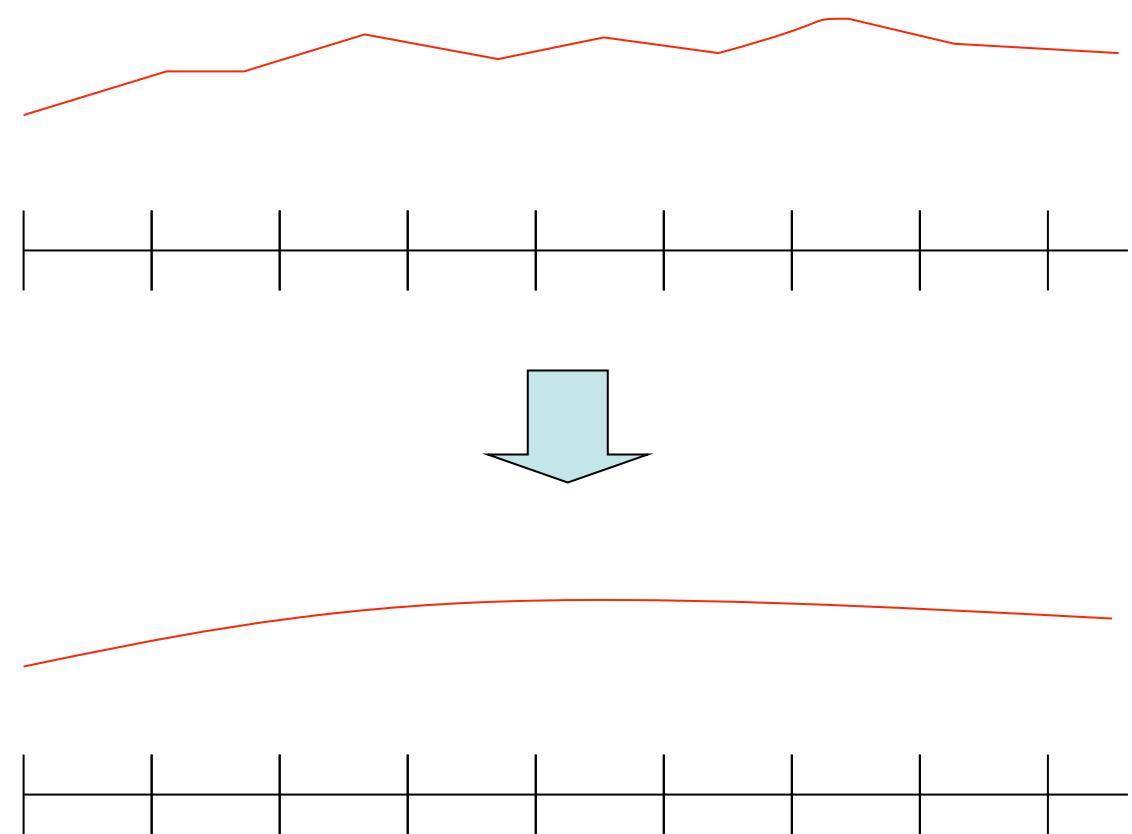
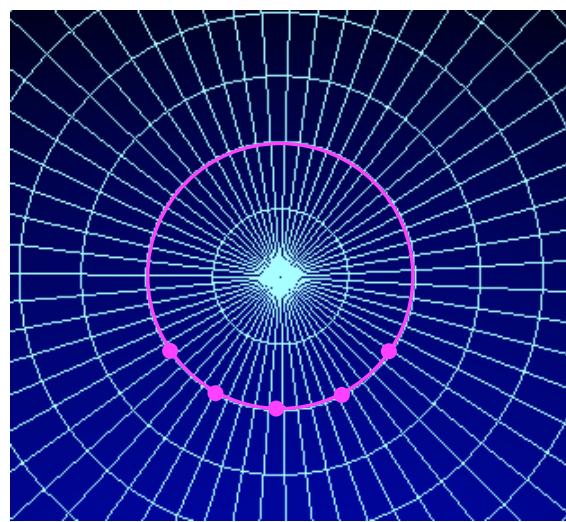
Grid Spacing Problem in Lat-Lon Grid

Severe CFL condition (short time step) near the poles.



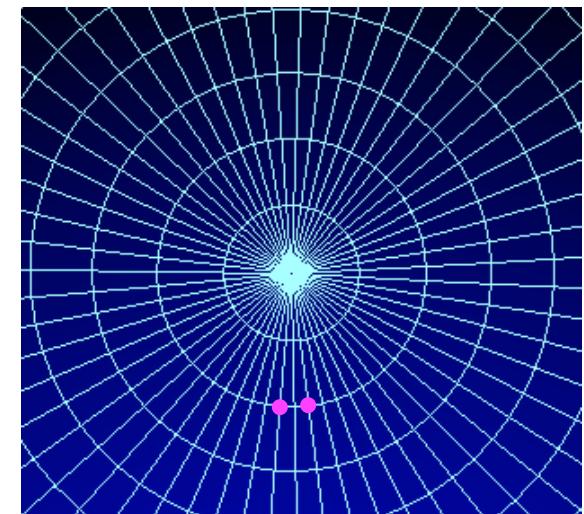
Spherical Filter

Retain the grids, but drop useless high wave number modes.
→ Filtering



Inefficiency of Lat-Lon Grid

- Too many useless grids in high-latitudes.
 - (1) Place many grid points near the poles.
(Spoiling the low-latitude's resolution.)
 - (2) Work hard to calculate data on the grids.
 - (3) Throw away most of the data!



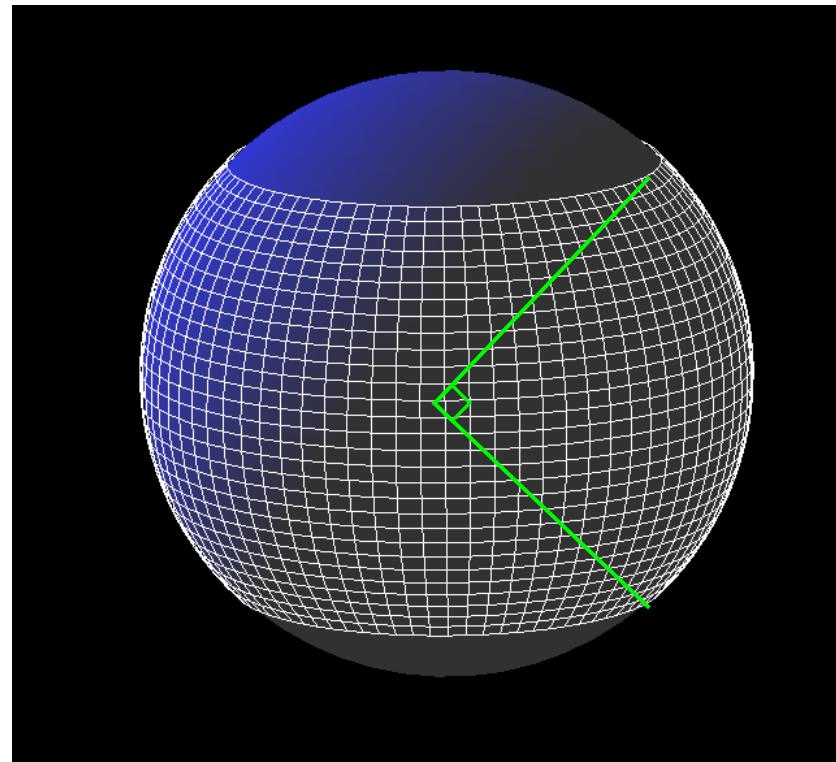
This is true for other spherical discretization methods:

- Double FFT spectral method (FFT both in latitude & longitude).
- Single FFT, hybrid method (FD in latitude & FFT in longitude).

Re-view the latitude-longitude grid

It is almost an ideal grid in the *low latitude region*.

- It is orthogonal coordinates (simple metrics)
- Nearly uniform grid spacing



Overset grid method applied to a sphere

- What is the simplest overset grid on a sphere?
 - Number of component grid = 2
 - The two component grids are the same

A baseball (or tennis ball)

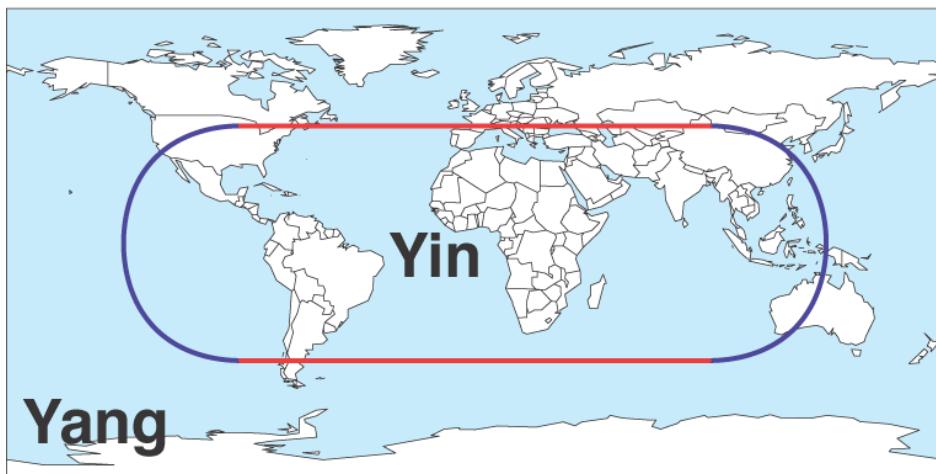
A spherical surface is covered by

- combination of two identical parts (patches).
- one seam.

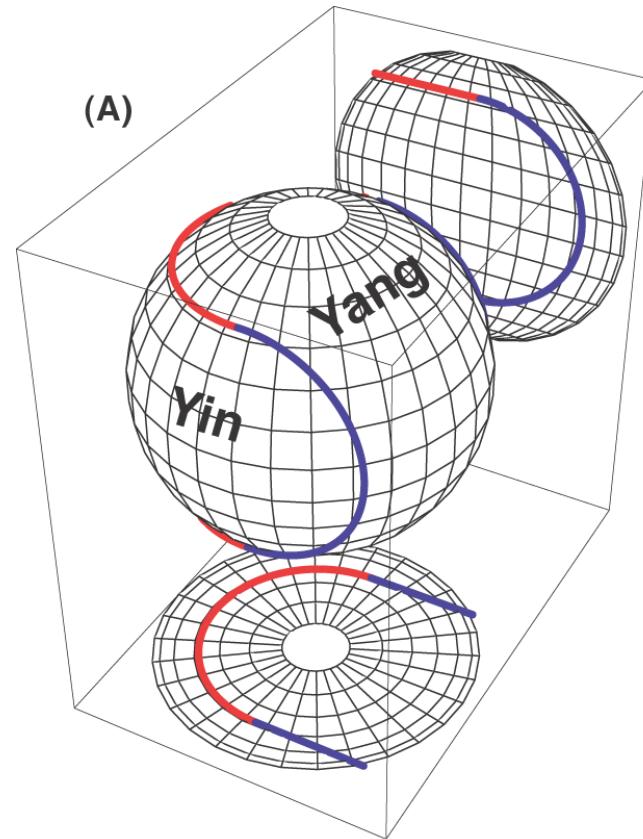


Dissections of a sphere into two identical parts

(A)



(A)



(B)



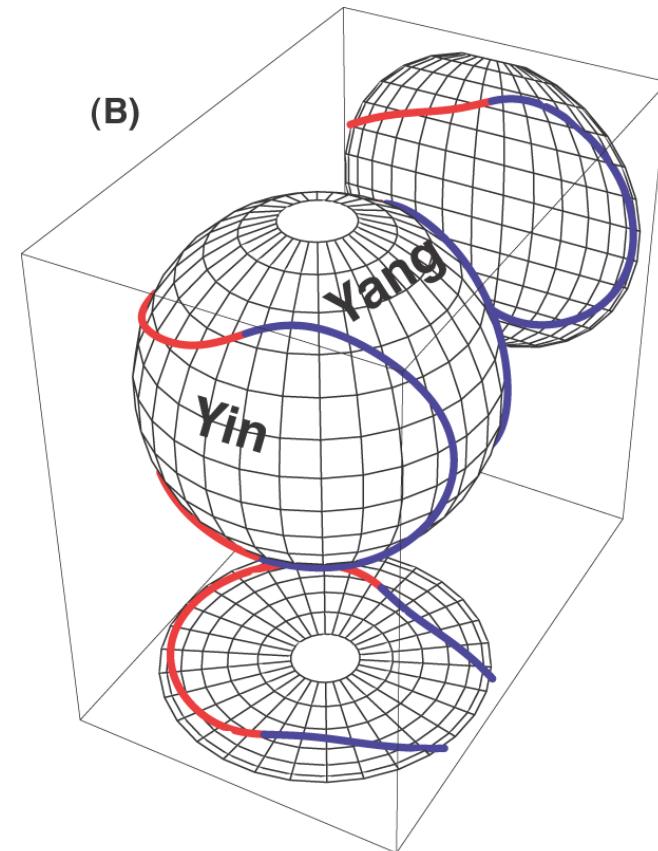
Yin-Yang 陰陽

Dissections of a sphere into two identical parts

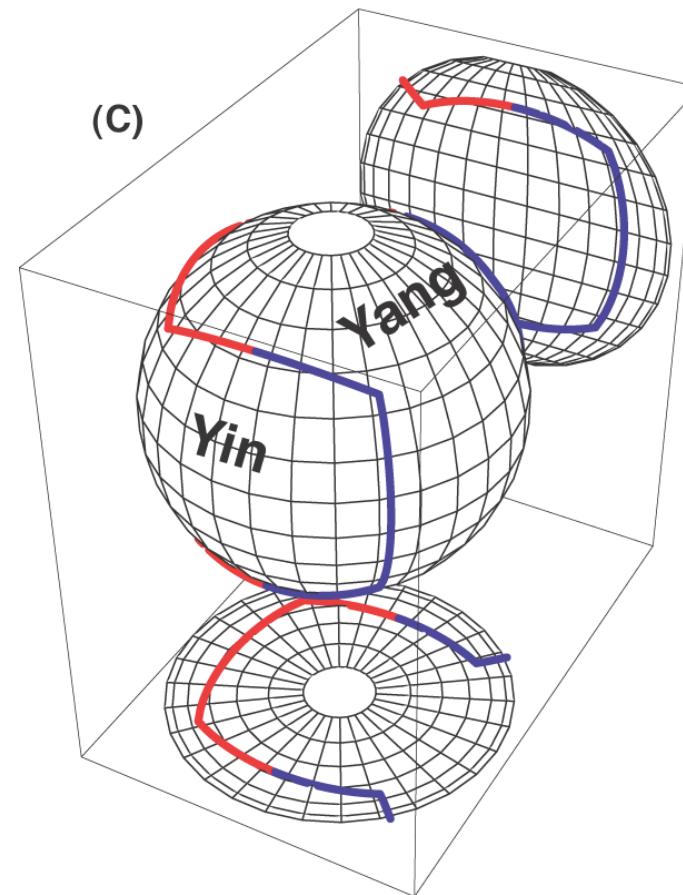
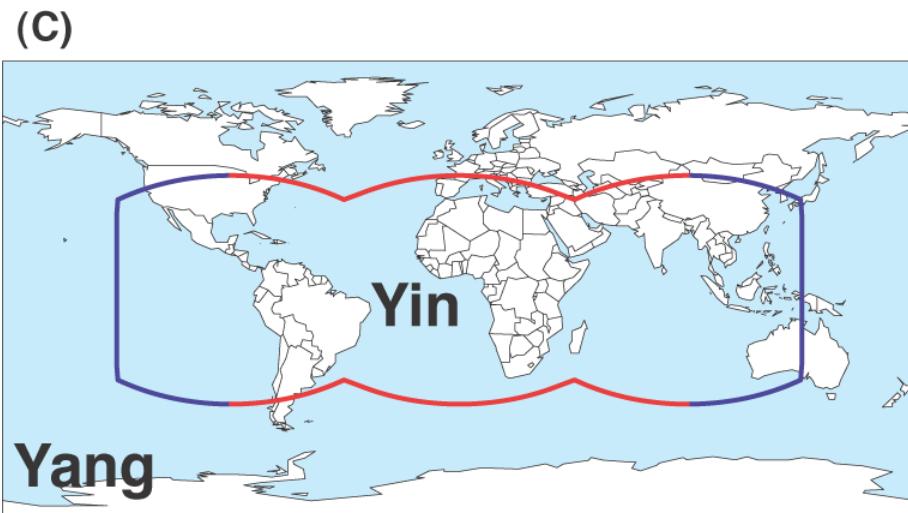
(B)



(B)

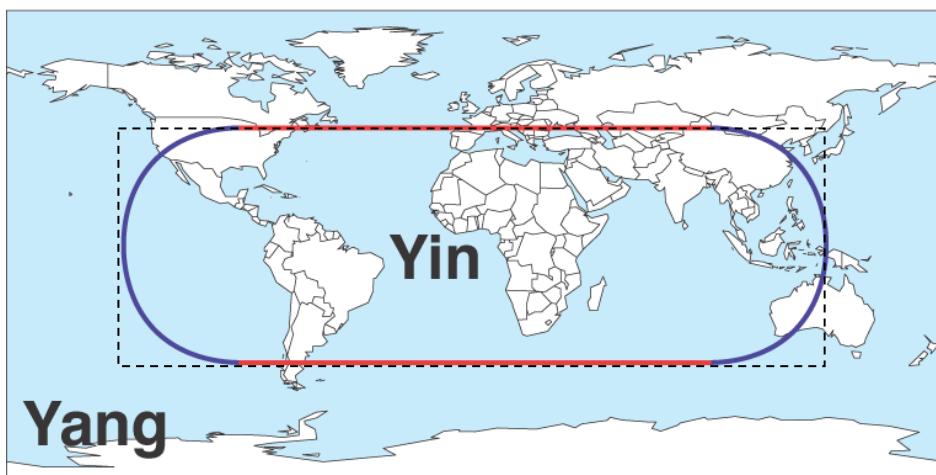


Dissections of a sphere into two identical parts

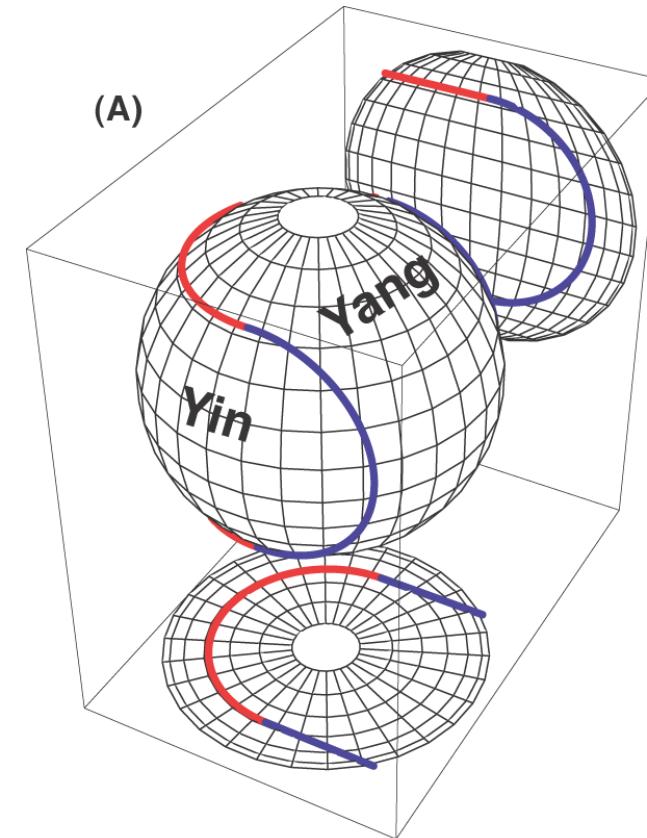


Dissections of a sphere into two identical parts

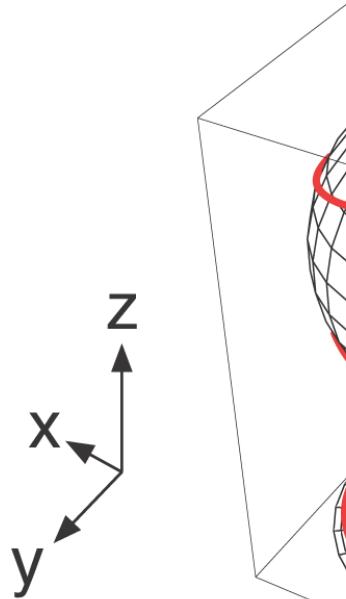
(A)



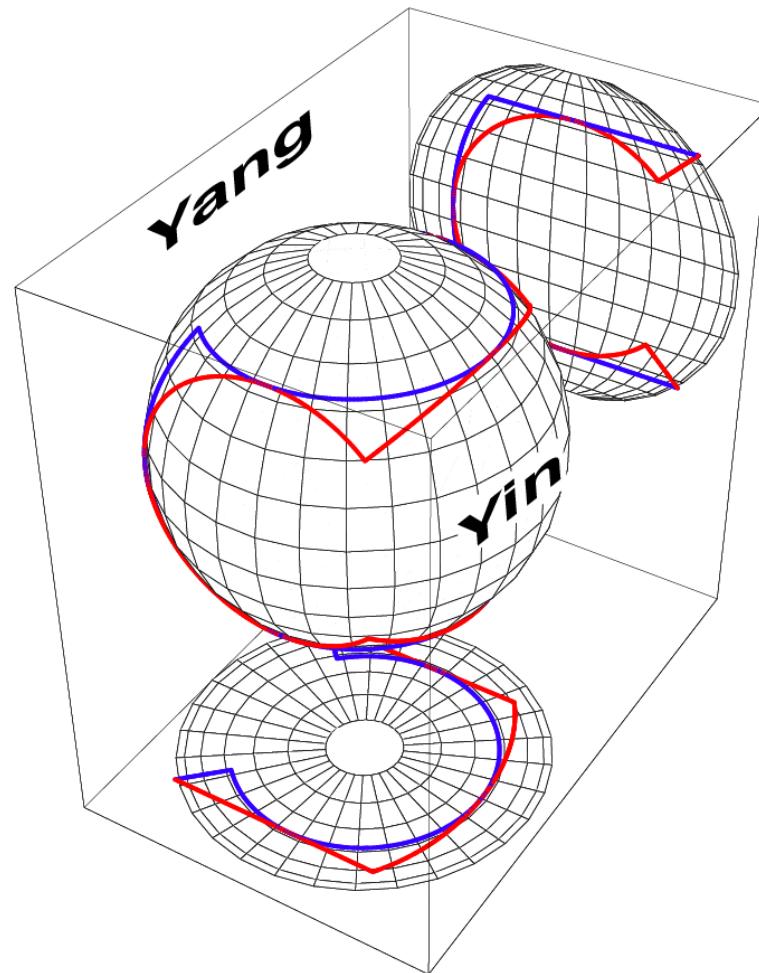
(A)



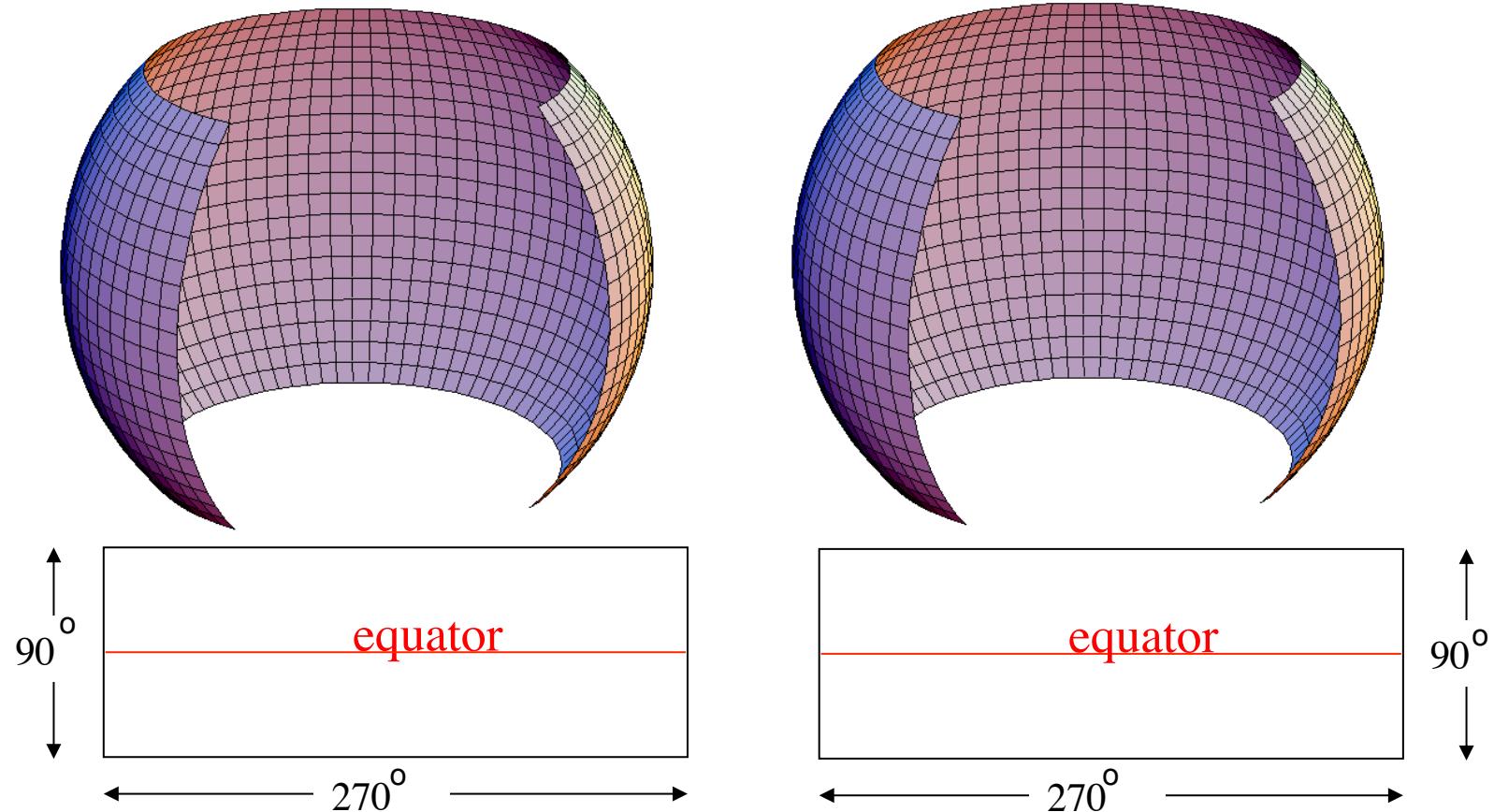
(B)



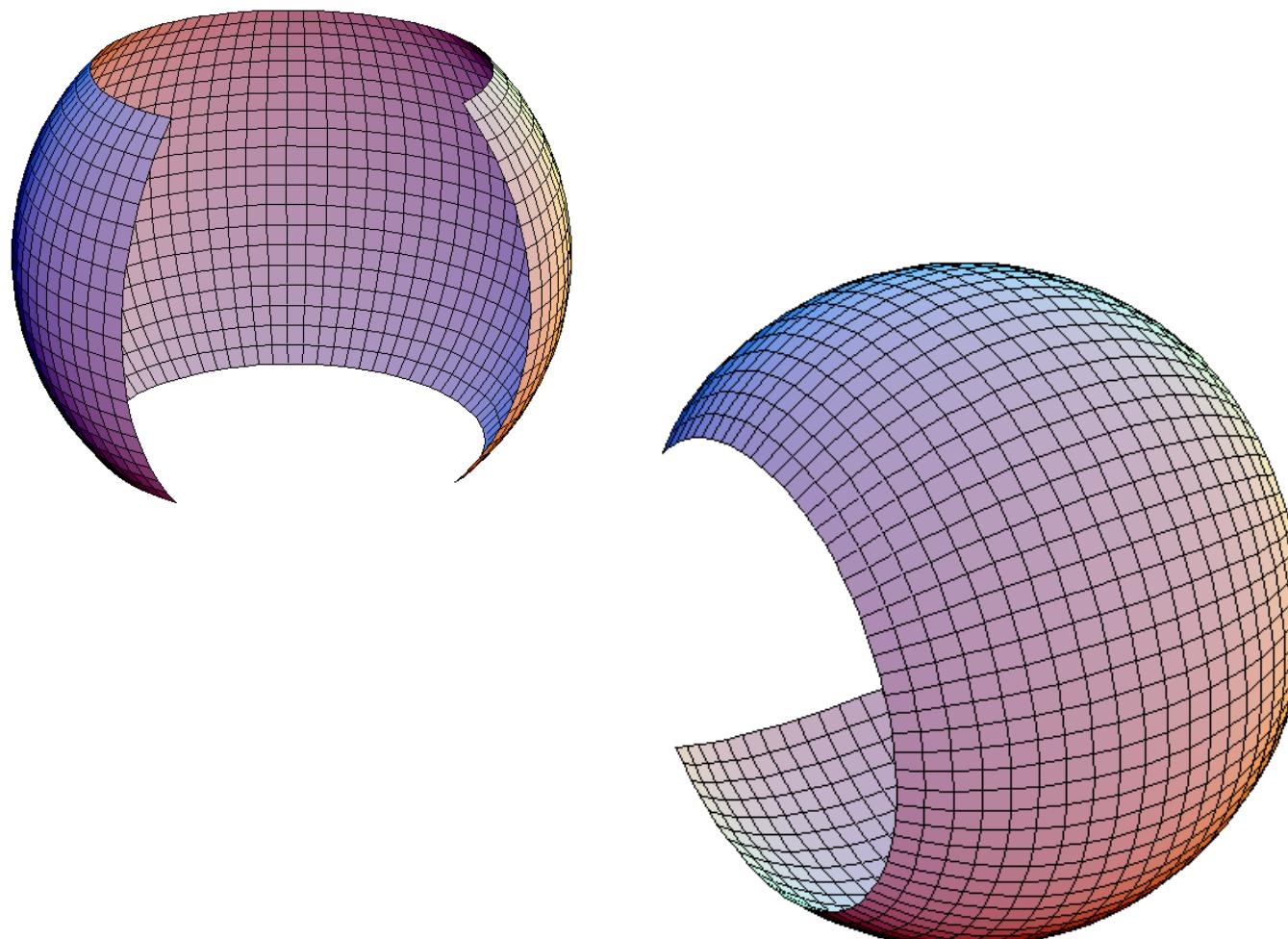
Spherical dissection with partial overlap



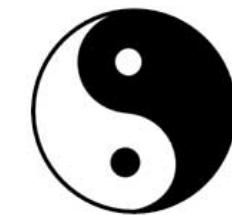
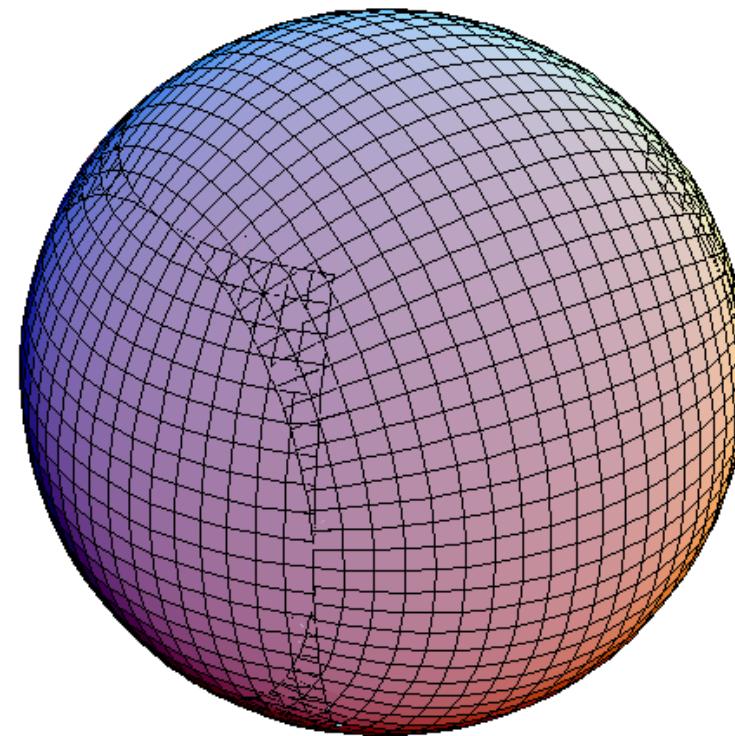
Combining two identical sub-grids to cover a full sphere



Combining two identical sub-grids
to cover a full sphere

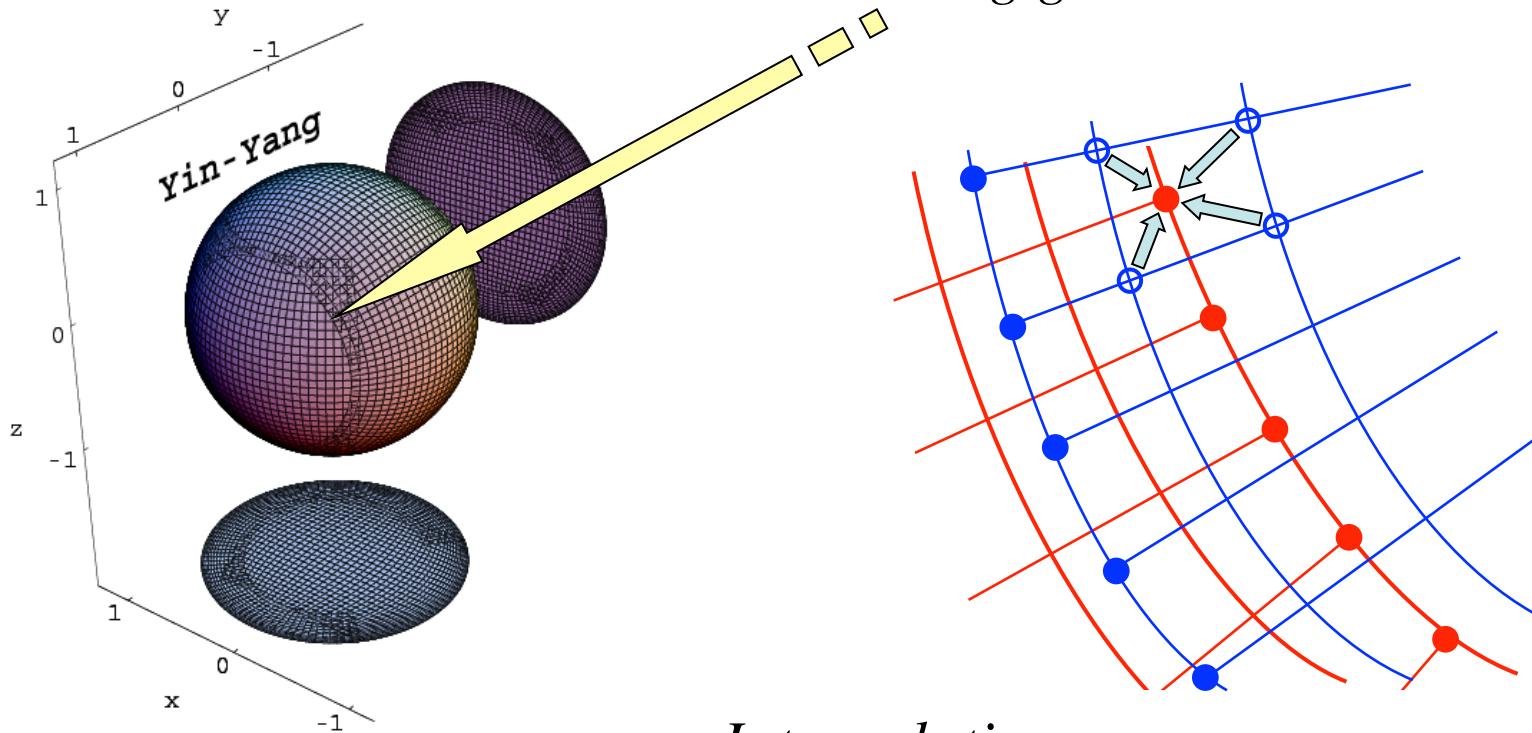


Yin-Yang grid



Yin-Yang 陰陽

Yin-Yang grid as an overset grid

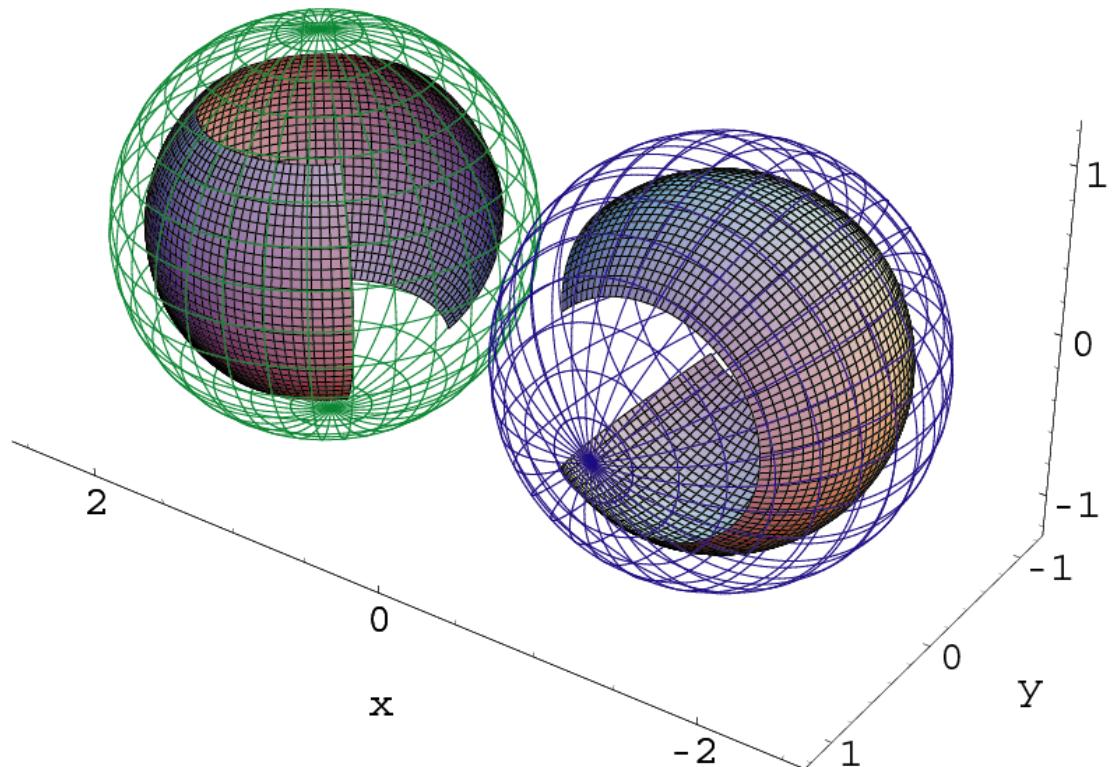


*Partial overlap
between Yin and
Yang grids.*

Interpolation
→ *boundary condition*

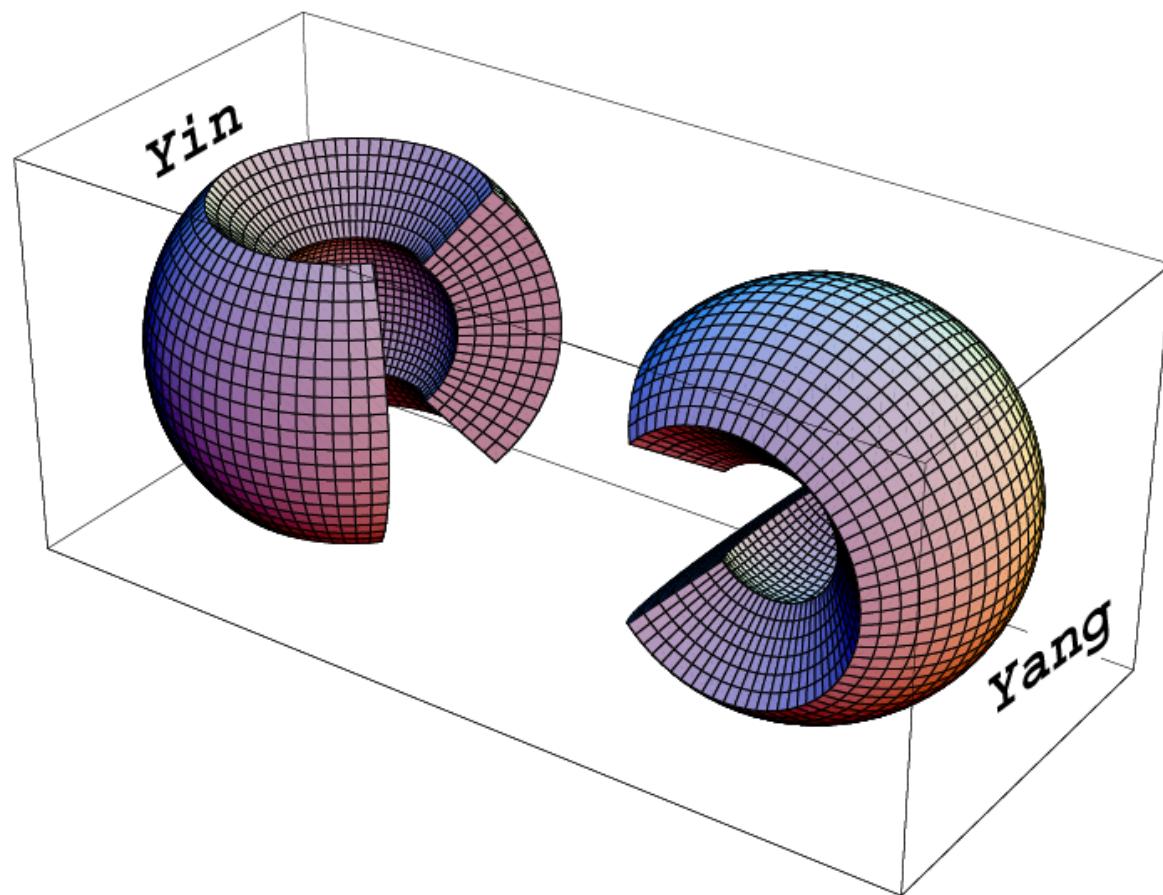
Concise coding of Yin-Yang grid:

- Make **one** routine on the (partial) latitude-longitude grid.
- Recycle it for **two times**; one for Yin and another for Yang.



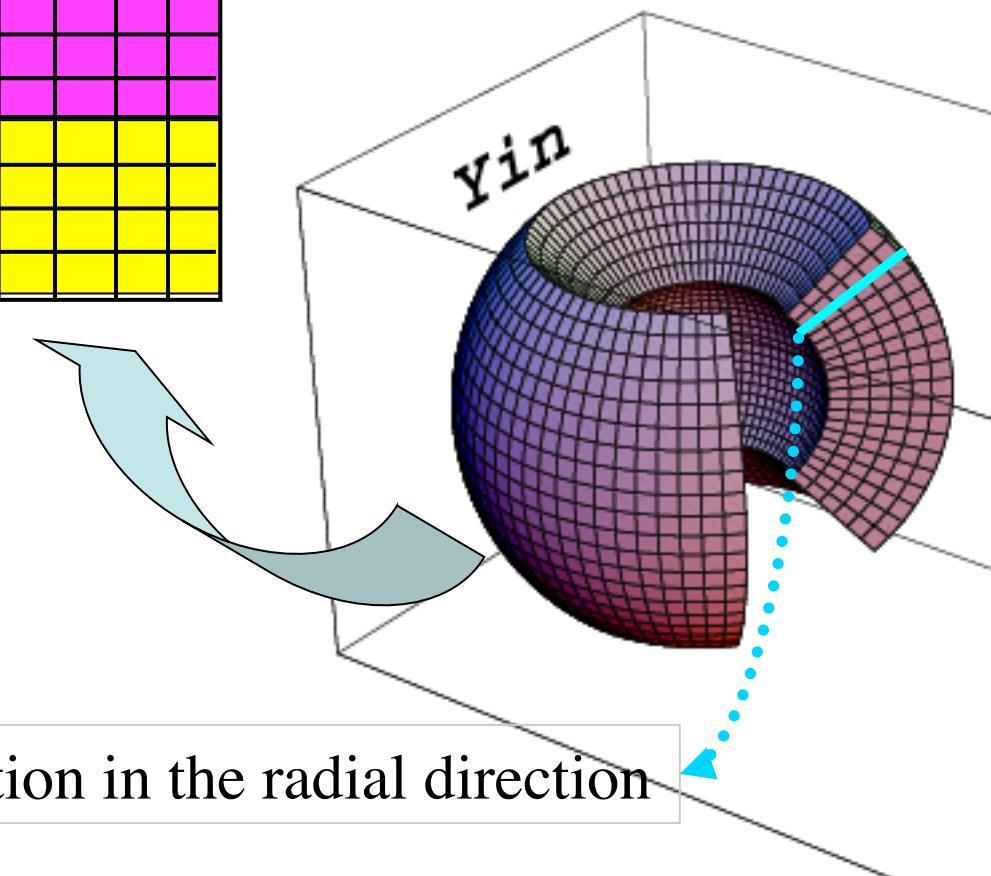
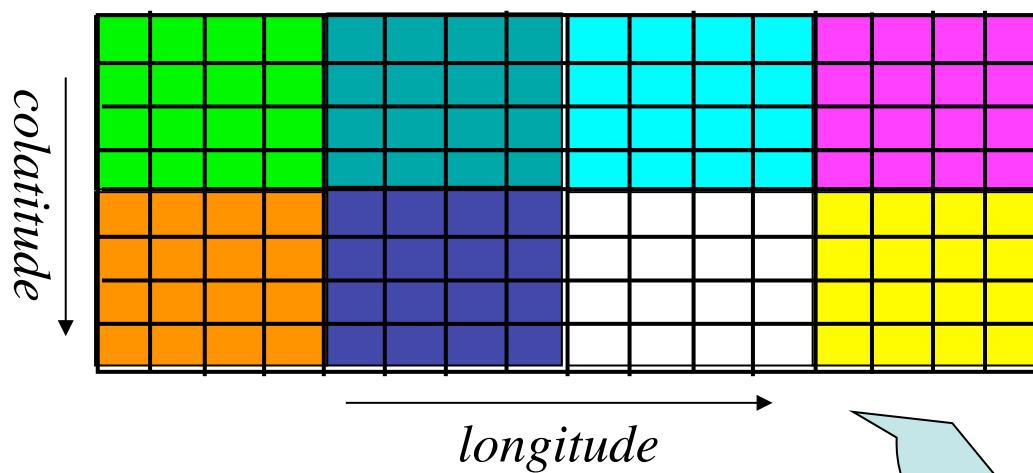
Routines for
- MHD solver
- boundary conditions
- interpolations

3-D Yin-Yang grid for spherical shells



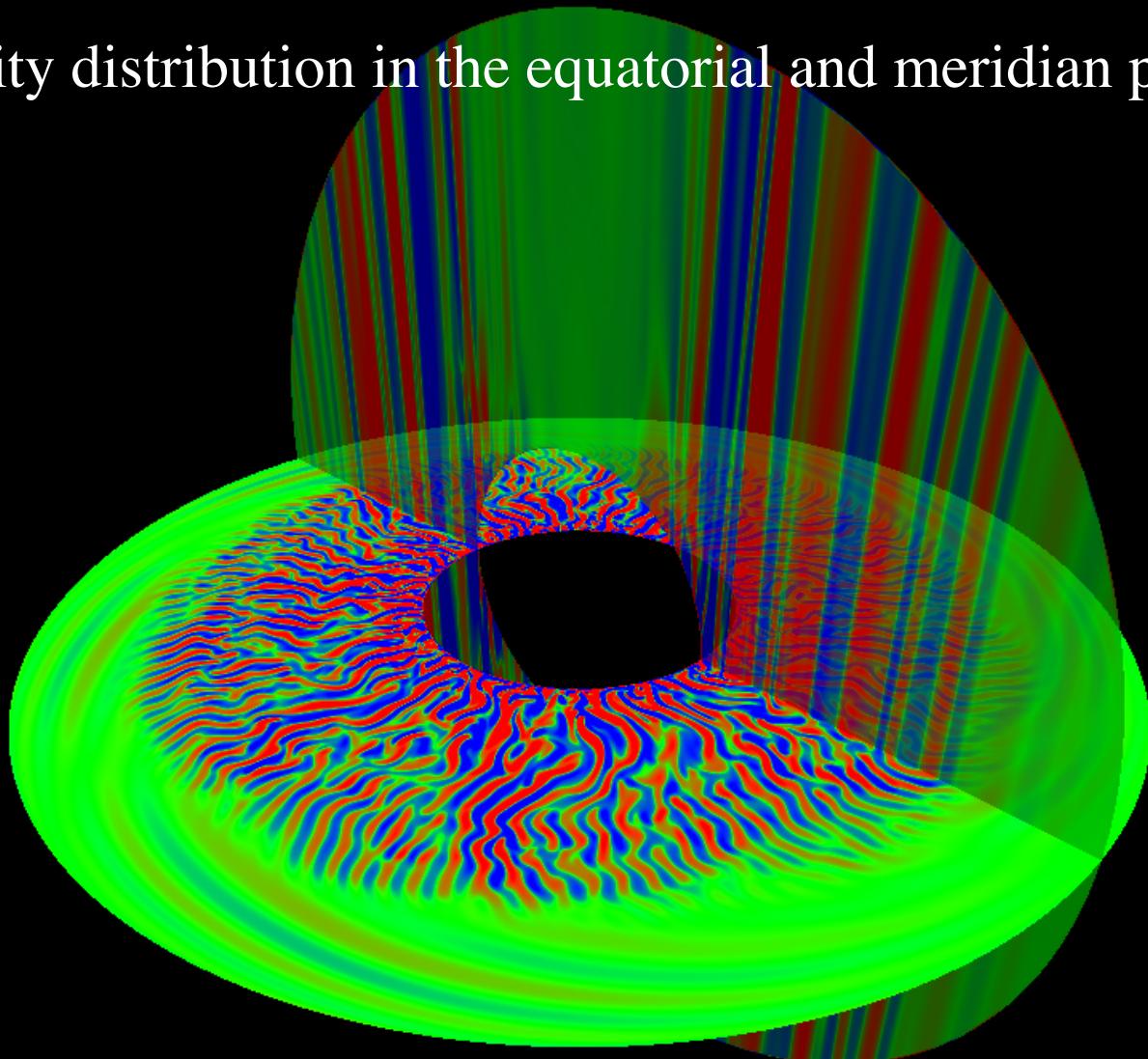
Parallelization on the Yin-Yang grid

2-dimensional domain decomposition
in the horizontal computational space.



Vectorization in the radial direction

Vorticity distribution in the equatorial and meridian planes



Sheet-like convection plumes

Summary

- Basic ideas of MHD simulation
- Many simple/sample/example codes.
- I'll make the source codes available for you.
- Check my lab's website:
URL: <http://www.research.kobe-u.ac.jp/csi-viz/>